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CTD Calibration and Processing Methods used at Woods Hole Oceanographic Institution

by

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1. Abstract

Processing methods, programs, and procedures currently used to create CTD data sets at Woods Hole Oceanographic Institution (WHOI) are described. The post-acquisition data processing steps include instrument calibrations in the laboratory and data calibration at sea, CTD data transformation from a time series to a pressure series, and the water sample data processing using the World Ocean Circulation Experiment (WOCE) format guidelines. Processing software has been developed for both the MicroVAX and IBM compatible personal computers. The description of the data processing procedures is restricted to the PC system. The programs are written primarily in FORTRAN with some format-related changes required between computer systems.

2. Introduction

In this report we detail the post-acquisition processing methods developed at Woods Hole Oceanographic Institution (WHOI) over the past fifteen years to handle the NBIS/EG&G Ocean Products Mark IIIb CTD data. We begin with a brief description of the lowered instrumentation including the water sampler, and the computer hardware necessary for data acquisition and processing. Next the WHOI CTD processing system is described from two perspectives. For the data user, we present the methodology used to transform CTD data from sensor measurements to processed observations, such as correction of pressure hysteresis and temperature corrections applied to pressure, lag correction techniques, oxygen algorithm, and so forth. For the data handler, we outline in the report and the appendixes the programs and the processing steps necessary to produce an archived CTD data set. The report covers only the CTD post-acquisition processing tasks, namely, those required to create a calibrated pressure series of temperature, salinity and oxygen values free of spurious observations, and a data file of associated water sample observations. The data acquisition is only briefly described in this report as more complete descriptions are found in references provided.

The CTD post-acquisition processing is divided into four stages:

- pre-cruise and post-cruise calibration of CTD sensors in the laboratory,
- water sample processing,
- data calibration at sea to water sample salinity and oxygens,
- and CTD data editing and processing to a uniform pressure series.

These four processing stages are interrelated and normally are performed in the order they appear in this report. First, the CTD laboratory calibration methods are reviewed. Next we discuss the water sample processing built around the water sample format developed for the World Ocean Circulation Experiment (WOCE) as described by Stalcup, et. al., 1990. The WOCE format accommodates not only salinity and oxygen but also nutrients, chlorofluorocarbons (CFC's), and various radioisotope tracers. The issues of data calibration at sea for salinity and oxygen follow. We then examine the processing methods used to edit and convert the CTD measurements into a uniform pressure profile of salinity and oxygen. Finally we describe the follow-up data quality control steps used to assure that data are well calibrated and free of errors.

A set of brief program descriptions can be found in Appendix 1. Readers, particularly those involved in data handling, will want to familiarize themselves with these program summaries in order to follow the data processing flow diagrams presented in this report. The programs, operating documentation, and test data files are available on 3.5

inch floppy disk on request from the authors for most of the PC programs listed in Appendix 1. For the most part programs described are written in FORTRAN-77, with the idea that FORTRAN promotes program portability.

We will not discuss the details of the CTD data acquisition systems in this report. Instead we provide the following brief overview of the two CTD data acquisition programs used at WHOI: CTDACQ which operates on MS-DOS PCs, and ACQUI which runs on Digital Equipment Corporations MicroVAX (μ VAX) computers under the VMS operating system. Both PC and μ VAX versions of the programs carry out the following tasks:

- storing all of the uncalibrated data as digitized by the CTD instrument to tape or disk;
- providing basic instrument quality control information to the user during the CTD cast via graphics plots and printer listings; and
- writing a subset of the CTD station data associated with water samples in a computer readable form.

Both the WHOI/URI-developed ACQUI μ VAX program and the EG&G-developed CTDACQ program provide capabilities for collecting, monitoring and storing data from EG&G/NBIS Mark IIIb CTDs, and both allow the user considerable flexibility in choosing instrument configurations and selecting variables to be displayed. Both acquisition programs have users' guides which document their capabilities (see Allen, 1992, and EG&G Ocean Products Software Manual).

The μ VAX program ACQUI stores the CTD data in CTD78 format (see Millard et al., 1978). The PC program CTDACQ stores CTD data in binary form with its own file format, and splits the calibration and header information into separate files (see Appendix 5 for examples).

3. Hardware Requirements

3.1 Lowered Instrumentation

The NBIS/EG&G Mark IIIb CTD underwater unit is equipped with pressure, temperature, conductivity and oxygen sensors. Other sensors can be added to the Mark IIIb CTD such as a transmissometer, a nephelometer, height-off-the-bottom detector, and a redundant temperature sensor. The NBIS Mark IIIb CTD telemeters data through a conducting cable in FSK (frequency shift keyed) format at 5000 baud to a deck unit which demodulates and converts it to a 9600 baud, RS-232 serial compatible data stream accessible through a serial computer port. As a data backup during the cruise, the original audio FSK CTD data signal is recorded on audio, or DAT, tape using commercially available cassette units. The CTD underwater unit has a hardware adjustable data length (in byte increments) to permit additional sensor data to be added to the telemetered data stream. A design goal of the data acquisition and processing programs on both the PC and μ VAX was ability to accommodate to an adjustable CTD data frame length. (A detailed description of the Mark III CTD can be found in the report by Brown and Morrison, 1978.)

A General Oceanics (GO) rosette fitted with Niskin bottles is used with the CTD for collecting water samples. At WHOI, the GO rosette is mounted approximately 1.5 meters above the CTD sensors, and creates a noticeble flow disturbance of non-oceanic conductivity/temperature structure during the up-cast profile. Because of wake-induced variations, normally only the down-cast is retained in the final CTD data set. The conducting cable is used for providing CTD power, telemetering data, and signaling the closure of the rosette sampler Niskin bottles. The CTD/rosette package is lowered at a descent rate near the package terminal velocity of between 1 and 2 m/s.

3.2 Seagoing Computers

The processing procedures have been adapted over the years to a variety of computers beginning with the H-P 2100 series mini-computers and the Scientific Data System (SDS) Sigma-7 main frame computer in the mid 1970's. The processing programs were converted to the VAX 11/780 VMS system in 1980, and to the μ VAX for seagoing processing by the mid 1980's. In the recent past, CTD data logging and processing have been adapted to the IBM MS-DOS compatible personal computer (PC).

The CTD data processing system, as described in this report, has been adapted to work on most IBM compatible PC's and has been tested on MS-DOS versions 3.2 through 5.0. A Digital Equipment μ VAX version of the CTD logging and processing system

has been tested on VMS operating systems 4.0 through 5.3. The minimum hardware requirements on either computer system are: an RS-232 interface port capable of 9600 baud, a hard disk (should have a minimum of 40 Mb on the PC and 71 Mb on the μ VAX), a removable disk or tape storage device, a printer, and a hard copy graphics device. We strongly recommend a spare data logging computer be available on all cruises.

3.2.1 PC-based Data Acquisition

The MS-DOS PC CTD data logging and processing system requires the following recommended minimum equipment installed on an IBM AT (80286) compatible computer:

640 kbytes installed Random Access Memory (RAM)

EGA (Enhanced Graphics Adaptor) or VGA card

EGA or VGA monitor

80287 Math co-processor

One - 1.2 Mb or 1.44 Mb floppy disk drive

One - 40 Mb hard disk drive

One - printer (graphics quality)

Two - RS-232 serial ports

In practice, the backup data acquisition PC is set up as a data processing computer, permitting acquisition and processing to occur simultaneously. The two computers are connected through a second RS-232 port allowing data to be passed between computers using a communications program such as LapLink[©]. Switch boxes are used to share the available RS-232 ports as shown in the PC computer system interconnection diagram of Figure 1.

3.2.2 MicroVAX-based Data Acquisition

The μ VAX data acquisition computer system is briefly described since it has been the primary seagoing data logging and processing computer system used at Woods Hole over the past few years. The data acquisition program requires at least a 71 megabyte disk for the VMS operating system, programs, and data storage, but a practical working disk size of 150 Mbytes is recommended for data acquisition and processing. In addition to

the operator console, four RS-232 ports are required. The incoming CTD data utilizes the first port. The second port is connected to a user terminal, the third port is connected to a printer, and the fourth port is connected to a plotter. The off-line mass storage is either a TK-50 streamer tape or a 9-track tape, or both. (See Allen, 1992 for further information on hardware and configuration requirements on the μ VAX.)

3.2.3 Hybrid System: MicroVAX and PC-based

In situations where both a μ VAX and a PC are available, the PC can be linked directly to the μ VAX either through an RS-232 port or through an ethernet connection. Note that ethernet requires an additional interface on both the PC and μ VAX. The PC can then serve both as a terminal for the μ VAX and as a data transfer link between the PC and the μ VAX. For data transfer the ethernet is preferred because it supports much higher (1 Mbyte/second) data transfer rates. With the hybrid system, data can be collected on the PC and then transferred either immediately or after some processing to the μ VAX for further processing and analysis. Many terminal emulation software packages provide graphics options to enhance the usefulness of the PC as a μ VAX terminal.

3.3 Shorebased Computer Requirements

The minimum shorebased computer requirements are identical to those of the seagoing μ VAX or PC system.

When the seagoing μ VAX is ashore, it may be "VAX clustered" with the VAXes at WHOI's central computer facility, thereby allowing easy access to a vast array of centralized computing resources.

4. Laboratory CTD Sensor Calibrations

The CTD/O₂ (Conductivity-Temperature-Depth-Oxygen) profiler requires accurate calibration of conductivity, temperature, and pressure sensors in the laboratory to provide state-of-the-art hydrographic measurements. This is particularly important in the deep waters (below 1500 meters) where the variations of temperature and salinity are small. The standard practice at WHOI is to calibrate the CTD pressure, temperature and conductivity sensors in the laboratory before and after each cruise against traceable transfer standards.

Calibrations are performed over the ranges of 0 to 6500 dbars. 0 to 30°C, and 20 to 60 milliSiemens per centimeter (mS/cm), respectively. The calibration procedure involves taking readings of the CTD sensor values and associated standard values at a sufficient number of intervals to describe any non-linearity of the sensors. This procedure documents the differences between the sensors and the standards. Normally, no actual adjustments to the sensor electronics are made as a result of these tests, because to do so would interrupt the instrument calibration history. It is recommended that the temperature and conductivity calibrations be performed with the instrument fully immersed in the calibration baths, and that the pressure transducer be calibrated at several different temperatures, in order to characterize fully the temperature sensitivity of each pressure transducer. All of the CTD sensors have been observed to drift with time (Millard, 1982), and for this reason frequent laboratory and or in situ recalibration is required.

4.1 Standards

The temperature standard at the WHOI Calibration Facility is a Yellow Springs Instruments platinum thermometer model number 8167-25 and an EG&G Ocean Products bridge model number ATB-1250 adjusted to a triple-point-of-water cell (at the triple-point temperature of 0.0100°C) and a melting-point-of-Gallium (ISOTEC model 17401) cell (at 29.7646°C, on ITS-90 Mangum, 1990). The conductivity standard is an EG&G model CSA-1250 conductivity bridge using a 5-electrode conductivity cell standardized with IAPSO Standard Seawater. The pressure calibration is performed with a deadweight tester connected to the CTD pressure port. WHOI uses a Ruska model number 4280-600 series deadweight tester (whose masses are checked periodically at the Massachusetts Bureau of Weights and Standards) with an accuracy of 0.01%.

There is currently no laboratory procedure employed for calibrating the oxygen sensor. In addition to the laboratory calibration standards, the CTD conductivity sensor and oxygen probe are both recalibrated on a regular basis at sea against water samples. The conductivity standard is again IAPSCO standard sea water while the water sample oxygens

are determined using a modified Winkler titration technique with an overall accuracy of 0.02 ml/l (Knapp et al., 1990).

The WHOI calibration facility's stated accuracy and resolution are shown in Table 1.

Table 1

Sensor	Range	Accuracy	Resolution	
Temperature	0 to 32°C	0.0015°C a	0.00001°C ^b	
Conductivity	0 to 100 mS/cm	0.0015 mS/cm ^c	0.000002 mS/cm ^b	
Pressure	0 to 10300 dbars	0.01%	0.0006 dbars	

^a accuracy limited by melting-point-of-Gallium cell accuracy

4.2 Temperature and Conductivity

There are two methods of laboratory temperature and conductivity calibrations employed at WHOI. One procedure is to immerse the CTD fully in a well-stirred bath with its sensors in close proximity to the temperature (ATB-1250) and conductivity (CSA-1250) transfer standards in an insulated, well-stirred salt water bath (normally at a salinity close to 35 psu) and to record values of the CTD and standards at a number of temperature and conductivity values. By varying the temperature of the bath, a temperature and conductivity calibration can be achieved, since changing the bath temperature also changes the conductivity. The CTD conductivity is calibrated against the CSA-1250, or measurements from salinity samples analysed on the Autosal 8400 then inverted from salinity to conductivity using the transfer standard temperature. This assumes that the 1978 Practical Salinity Scale (PSS78) is valid for the bath water, which may not be correct for artificial seawater made from commercial sea salts such as used at WHOI.

An alternative temperature calibration method involves using several (five are used at WHOI) Tronac constant temperature baths maintained at different temperatures and sequentially immersing the sensors and lower quarter of the CTD in each bath. This method, although quicker than the fully immersed calibration, should not be used as a substitute, as it may not "calibrate out" temperature effects in the CTD's electronics.

c accuracy tied to IAPSCO water at 0.001 practical salinity units (psu) and bath stability

^b EG&G ATB/CSA-1250 temperature/conductivity bridge

For this reason, the method of full immersion is preferred for temperature calibrations. It should be noted that comparing the readings from both fully and partially immersed calibrations may help isolate certain electronics problems.

An alternative conductivity calibration technique employed at WHOI involves setting up several room temperature salt water baths at various salinities from 15 to 40 psu and again moving the CTD sensors and CSA-1250 conductivity probe between baths. We have found that this conductivity calibration yields a more reliable conductivity calibration, particularly for conductivity sensor bias determination and for this reason, is preferred over the fully immersed method.

The number of standard and CTD sensor observation pairs recorded over the sensor range of each variable depends on the linearity of the sensor. Typically, values of temperature are recorded every 5°C between 0 and 30°C and conductivity every 10 mS/cm from 20 to 60 mS/cm.

4.3 Pressure

The pressure calibration is done by coupling a deadweight tester (DWT) to the pressure port of the CTD and recording the values of the CTD pressure, together with that of the standard, over the range of the CTD sensor. The pressure calibration is always recorded while both loading and unloading the DWT, and is usually repeated for at least one other temperature. Room temperature changes are recorded using a separate mercury thermometer in order to make corrections to the DWT, as discussed below. For the recently implemented titanium pressure transducer (Millard et al., 1992), a separate internal temperature sensor inside the pressure transducer is measured, and this temperature must stabilize and be recorded to make a complete CTD pressure measurement. Pressure data are typically recorded at 0, 500, 1000, 2000, 3000, 4000, 5000, 6000, 7000, 8000 and 9000 psi, during both loading and unloading of the DWT normally at both room temperature and the ice point.

To correct the deadweight tester values from the nominal DWT pressure, a series of conversions and corrections are required. The corrections must be applied to the DWT pressure value to obtain an accuracy of 0.01 percent for the Ruska model 4280-600 Deadweight Tester. If necessary, the conversion factor from psi to dbar of 0.68947572 psi/dbar is applied. The corrections (which are discussed further by Fofonoff et al., 1974) include:

- (1) local gravity correction from standard gravity = 9.80665 m/s^2 ,
- (2) air buoyancy correction to the weights,
- (3) fluid head offset correction,

- (4) correction for thermal expansion of the piston,
- (5) correction for elastic distortion of the piston with loading, and
- (6) atmospheric pressure.

An accurate measurement of pressure is particularly important for CTD salinity measurements, because an error of 2.5 dbars produces an error not only in the vertical position of the measurement but also in the calculated salinity (of 0.001 psu) and density.

4.4 1990 International Temperature Scale Considerations

After 1 January 1990, JPOTS (1991) recommends that temperatures be reported on the ITS-90 International Temperature Scale of 1990 (T_{90}). When using ITS-90, one needs to keep in mind that the algorithms for computing the physical property of seawater (Fofonoff and Millard, 1983) were developed on the earlier IPTS-68 International Practical Temperature Scale of 1968 (T_{68}). The distinction between these two temperature scales is discussed by Saunders (1990) and Fofonoff and Millard (1991). The latter reference also discusses the implications of this temperature scale change on the calculation of various physical properties of seawater. The change of temperature scale particularly affects the calculation of salinity from conductivity (using the Practical Salinity Scale of 1978, PSS-78), as well as the inverse calculation of conductivity from salinity.

For purposes of these calculations, the following formula is used to convert T_{90} to T_{68} :

$$T_{68} = 1.00024 \cdot T_{90}. \tag{1}$$

During the laboratory and at-sea calibration of conductivity, the associated temperature must be converted from ITS-90 to IPTS-68 before inverting conductivity from salinity using PSS-78. See the discussion by Fofonoff and Millard (1991).

4.5 Fitting the Calibration Data

The best fit NBIS/EG&G Mark IIIb CTD sensor calibrations are usually found to be linear in conductivity (with a typical standard deviation of 0.001 mS/cm), quadratic in temperature (with a typical standard deviation of 0.0005°C), a third order polynomial in pressure for the stainless steel pressure transducer, and a quadratic for the titanium pressure transducer (Millard et al., 1992). Both pressure transducer polynomials describe the

calibration data with a typical standard deviation of less than 0.3 dbars. The polynomial coefficients to calibrate the raw sensor data are determined using standard least squares techniques (program LABCAL1 described in Appendix 1). When fitting the laboratory calibration data, a manual editing procedure is used to remove suspect calibration values (i.e. those with a large difference from the polynomial) before refitting. The coefficients are stored in an instrument calibration file for use with the acquisition and post-processing programs. A combination of pre-cruise and post-cruise laboratory calibration data is frequently used to establish final pressure and temperature calibration coefficients. The stainless steel pressure transducer requires separate polynomials for the loading (downtrace) and unloading (uptrace) in order to apply the pressure hysteresis correction that follows.

Subtle instrument problems are often identified by careful examination of CTD calibrations prior to a cruise. Large shifts of calibration or fits requiring a higher order polynomial than normally required to reduce residual variance indicate instrument malfunction or poor calibration data. The most recent calibrations of an instrument should always be compared with the previous calibration history.

4.6 Conversion to Engineering Units

Polynomials are used to transform raw instrument measurements (with subscript r) of pressure (P), temperature (T), and conductance (G) to engineering units.

$$P = E_0 + D_0 \cdot P_r + C_0 \cdot P_r^2 + B_0 \cdot P_r^3$$
 $T = E_1 + D_1 \cdot T_r + C_1 \cdot T_r^2$
 $G = E_2 + D_2 \cdot G_r$

The titanium pressure requires only a second order polynomial but requires additional temperature corrections as discussed by Millard et al. (1992).

All programs correct the measured CTD conductance G to conductivity C using the cell material deformation correction formula:

$$C = G \cdot [1 + \alpha \cdot (T - T_0) + \beta \cdot (P - P_0)]$$
 (2)

where the coefficients for alumina are

$$\alpha = -6.5 \text{ E}^{-6} {}^{\circ}\text{C}^{-1}$$

 $\beta = 1.5 \text{ E}^{-8} \text{ dbar}^{-1}$
 $T_0 = 2.8 {}^{\circ}\text{C}$
 $P_0 = 3000 \text{ dbar}$

and P, T, and G are CTD measured pressure, temperature, and conductance.

4.7 Pressure Hysteresis Correction

The pressure loading (downtrace) and unloading (uptrace) calibrations typically show sensor hysteresis differences of between 5 and 8 dbar for a stainless steel CTD pressure transducer (Millard et al., 1992). Importantly, the pressure errors incurred on the uptrace are a function of the maximum pressure of the cast. An uptrace pressure calibration algorithm is derived for each cast by combining the laboratory-derived loading P_{dn} and unloading P_{up} polynomials. The stainless steel transducer hysteresis is compensated for using the following equation:

$$P = P_{up} \cdot (1 - W) + P_{dn} \cdot W \tag{3}$$

$$W = e^{-(P_{bottom} - P_{dn})/Z_0} \tag{4}$$

where

P is the derived uptrace pressure,

 P_{up} is the pressure value scaled with the uptrace calibration polynomial,

 P_{dn} is the pressure value scaled with the downtrace calibration polynomial,

P_{bottom} is the maximum pressure of the station, and

 $Z_0 = 300 \text{ dbar.}$

The hysteresis correction model for the stainless steel pressure transducer given in equation 3 matches the downtrace and uptrace pressures at the bottom, and then exponentially decays from the down pressure calibration curve to the up calibration curve over a scaling length Z_0 .

The hysteresis correction is not necessary when the CTD uses a titanium pressure transducer. Instead, a set of static and dynamic temperature corrections is required, as

discussed by Millard et al. (1992). Over the past year, most WHOI Mark IIIb CTD's have been retrofitted with titanium pressure transducers.

The correction to the stainless steel pressure sensor for the variation of CTD on deck pressure from station to station by adjusting the pressure bias has been found to be important. We don't have enough experience with the titanium transducer to know if there is a non-temperature related pressure bias change from station to station.

4.8 Laboratory Calibration Data Flow

Calibration data are manually entered into an ASCII file whose name includes instrument number, version letter, and calibration date in the form *invmmmyy*.CAL. For example, 11CSPT88.CAL identifies a conductivity (v = C) calibration file for CTD#11 with a September 1988 calibration date. A complete description of the file naming conventions is given in Appendix 2. The CTD laboratory calibration data flow is shown in Figure 2. The program LABCAL1 is used to determine the least squares regression (LSR) polynomial coefficients relating the CTD sensor measurements to laboratory standards values. The coefficients are stored together with residuals in an output file having the same input file name but a new file extension, *iivmmmyy*.FIT. A file may also be created containing differences between calibration standard and CTD values for each parameter stored in an output file again having the same input file name, but with another file extension, *iivmmmyy*.DIF. Several *iivmmmyy*.DIF files for a particular sensor created on various dates can then be plotted together using commercial plotting software (such as GRAPHER ©) to view the drift in the sensor, as shown in the case of temperature in Figure 3.

5. Water Sample Post-Processing

A General Oceanics rosette multi-bottle sampler is used to collect water samples. The water bottles usually are closed at depth levels selected based on scientific merit. For calibration purposes, it is useful for the water samples not to be weighted toward either shallow or deep observations. A random distribution with pressure and temperature would be well suited for calibrations. Water samples are currently collected on the upcast to prevent sample contamination from bottle leakage.

The water sample data processing system is designed to achieve two objectives. One is to assemble and archive the various water sample observations with associated CTD measurements in the WOCE water sample format (see Joyce et al., 1991). The second objective is the determination of CTD conductivity and oxygen sensor calibrations. To

achieve these objectives, separate data archives are required, as the CTD conductivity and oxygen sensor calibration task requires unscaled CTD measurements such as conductivity, oxygen current and oxygen temperature, which are not stored in the WOCE water sample archives.

5.1 Water Sample Data Processing Flow

Both the PC and the μ VAX acquisition programs allow the operator to create a file of CTD observations at the time of bottle closures. The CTD data acquisition program writes averaged values of the raw, uncalibrated CTD/O₂ sensor data representative of each bottle closure to a water sample data file. The format of the PC and the μ VAX acquisition bottle files differs, and therefore a reformatting step is required to create a common bottle file format. The bottle data reformatting and the water sample processing steps, beginning with BTLEXTR, are shown in Figure 4 for the PC. After reformatting, the water sample data processing steps and programs are identical on both the PC and VAX computers but file naming conventions differ (see Appendix 2 for file naming and letter designator interpretation). The PC file naming convention is followed throughout this report. The processing sequence shown in Figure 4 accomplishes the following: the unscaled data file from BTLEXTR is scaled to engineering units with program WOCETMPL which outputs data in the WOCE water sample format file ssccvttt. TMP. This file is then passed on to the hydrographic group. They support a program (MERGE in Quick Basic) to merge in water sample salinities and oxygens from the Autosal and Winkler titrations. The file of water sample salinities and oxygens is then returned to the CTD processor and remerged with the unscaled CTD data in the bottle file using program BTLMRG. Later, a series of these files is merged together to be used for determining CTD conductivity calibration coefficients with programs CONVERT and CONCALD as discussed in the next section. Appendix 3 further illustrates the calibration steps together with the data files required.

The water sample collection procedure currently used at WHOI involves stopping the CTD/rosette package on the upcast. It is difficult to form oxygen calibrations from these stopped upcast observations as the polarographic oxygen sensor on the CTD does not perform well at low flushing rates. A program OXUPDATE has been developed for merging by pressure the downcast CTD observations with the upcast water sample oxygens. OXUPDATE requires the file *sscciill*.OXY from the oxygen calibration procedure discussed later.

After the CTD conductivity and oxygen sensor calibrations have been established (see next section), program WOCETMPL is used to produce a second WOCE water sample data file (Figure 4) with refined CTD salinity and oxygen values. The output file extension given to this best CTD salinity and oxygen calibration file is ssccvttt.CTP. The file ssccvttt.TMP is also distributed to other chemical analysis groups which merge their

data into this WOCE format data file. Program SEAMERGE (not indicated on Figure 4) merges the various groups' water sample data into a single file.

5.2 Water Sample Data Evaluation

Plots of CTD and water sample salinity and oxygen versus potential temperature are used to quality-control the conductivity (salinity) and oxygen data. An example of a potential temperature versus salinity plot is shown in Figure 10 and discussed in Appendix 4. Another quality control of the CTD salinity and oxygen calibrations involves plotting differences of the CTD and water sample observations versus station number and pressure. Examples of these plots can be found in Figures 8, 9, 11, and 12 which we discuss in Appendix 4 for conductivity and oxygen respectively. On the PC, the program WS_PLOT is used to create a file which is compatible with the commercial program GRA-PHER ©. Comparisons can be made directly of the CTD and water sample salinity and oxygens using the observations in the properly calibrated WOCE water sample data file.

6. Data Calibration at Sea

6.1 General

Before CTD data is converted to engineering units, the conductivity and oxygen sensor calibrations must be established. The calibration of conductivity (salinity) and oxygen requires using the *in-situ* water sample salinity and oxygens as both of these sensors can drift significantly over the course of a cruise.

An iterative fitting procedure has been developed for determining both conductivity (salinity) and oxygen algorithm model coefficients. The water sample derived values are subtracted from the CTD/O_2 sensor modelled values after adjusting the coefficients of the model to minimize the sum of squares of these differences (residuals). Individual differences between water sample values and the sensor model are checked against an edit criterion involving the product of the standard deviation of the residuals and an edit factor (F). The edit factor (F) is chosen to minimize the probability of rejecting valid observations consistent with eliminating bad data. For residuals with a normal distribution, a value of F = 1.96 has a 5% chance of rejecting good values while F = 2.6 has a 1% and F = 3.3 has a 0.1%. The default factor of 2.8 has a 0.5% chance of rejecting good data for a normally distributed process. After removing outlying data, the remaining data are refit in an identical fashion. The process is continued until no further observations are rejected.

6.2 Conductivity (Salinity) Sensor Modelling

In order to determine the CTD conductivity sensor calibrations, the water sample salinities must be converted to *in-situ* conductivities C_w . This requires accurate temperature and pressure values corresponding to the water sample salinity observations and therefore the best calibrated CTD temperature and pressure are used. The water sample conductivity is obtained using the FORTRAN routine SAL78 described by Fofonoff and Millard (1983):

$$C_w = SAL78 (S_w, T, P, 1)$$

where S_w is the water sample salinity and C_w is its corresponding *in-situ* conductivity. (The argument list of function SAL78 ends with a flag which equals 1 to indicate inversion of salinity to conductivity.) A value for conductivity at p = 0.0 dbars, S = 35 psu, and t = 15°C of $C_{35,15} = 42.914$ mmho/cm is used to convert conductivity ratios of PSS-78 to conductivity. The raw CTD conductivity G_r is corrected for the materials deformation given in Equation 2. The model for determining CTD conductivity includes a linear station dependent drift to allow correction for coating (or cleaning) of the cell by foreign material. Normally a positive adjustment is required which represents conductivity cell coating. The conductivity sensor model C_m is

$$C_m = G_r \cdot (D_2 + H \cdot N_o) + E_2.$$
 (5)

 D_2 and E_2 are conductivity slope and bias adjustments, following the notation of section 4.6, and H is a station-dependent conductivity slope adjustment multiplying station number N_o . The conductivity bias can be fixed or varied and the station-dependent slope H is optional. One or more of the model coefficients are varied to minimize the residual variance σ^2 defined as

$$\sigma^2 = 1/N \sum (C_w - C_m)^2.$$
 (6)

The editing procedure for removing outlying data involves the following test on the residuals to insure that no residuals fall outside the edit bounds. Again, the default edit factor F is 2.8.

$$|(C_{w} - C_{m})| > F \cdot \sigma \tag{7}$$

6.3 Conductivity Calibration Processing

Before the conductivity calibration can take place, the water sample salinities must be merged into the raw bottle file as discussed earlier in section 5.1. The program CON-VERT is then run to scale the raw CTD bottle observations to engineering units using the instrument calibration file. CONVERT takes data from the combined station water sample file (sscciill.LST) and converts it to engineering units except for conductivity which is scaled with a nominal slope adjustment value of 0.001. The input file must only contain CTD data from a single CTD instrument. The water sample salinity is inverted to an in-situ conductivity using the CTD pressure and temperature data. The conductivity calibration sequence is depicted in Figure 5. The program to fit the CTD conductivity to the water sample derived conductivity, CONCALD, allows the user to determine the CTD conductivity polynomial coefficient(s) of bias/slope or slope with user supplied bias. It also allows a station varying slope. CONCALD produces three output files indicated in Figure 5. These are: the conductivity calibration coefficients and the histogram of the distribution of residuals stored in the file (sscciill.HIS.); a file of rejected data (sscciill.REJ); and finally a file of acceptable data which are included in the final fit (sscciill.RES). An outline of the conductivity calibration steps with input and output files is given in Appendix 3. Examples of the various input and output files can be found in Appendix 4.

When looking at the conductivity (and also oxygen) residuals in both the sacciill.RES and sacciill.REJ files, one must keep in mind that the residual is a difference between CTD and water sample values. Because the CTD conductivity calibration tends to be stable in time, our experience has been that the sacciill.REJ file normally contains questionable water samples and we use this file during a cruise to identify leaky rosette bottles. The vertical separation of the rosette bottles and CTD sensors (approximately 1.5 meters for the WHOI package) can introduce systematic errors in regions of strong vertical salinity gradient. At present, we do not correct for this height difference and therefore, data from strong vertical gradient regions of both salinity and oxygen should be excluded when data are used for calibration.

6.4 Oxygen Sensor Modelling

The oxygen model has the following form (Owens and Millard, 1985)

$$OX_m = A \cdot (Oc + B \cdot \frac{dOc}{dt} + C) \cdot OXSAT(S,T) \cdot e^{D \cdot [T+E \cdot (T_o-T)]+F \cdot P}$$
 (8)

where A is the slope, B is the time constant for oxygen diffusion through the membrane, C is the oxygen current bias, D is a temperature correction [TCOR], E is the weighting

factor of oxygen sensor and water temperatures [Wt], F is the pressure correction [PCOR], Oc is oxygen current, T_o is the oxygen sensor temperature, OX_m is the computed CTD oxygen, and OXSAT(T,S) is the oxygen saturation value after Weiss, 1970. A more recent oxygen saturation algorithm has been developed by Benson and Krause (1984) and has the JPOTS endorsement.

Fitting the coefficients of the oxygen model requires a non-linear regression technique. We use an algorithm found in *Numerical Recipes* (Press et al., 1986) to minimize the residual variance with respect to one or more of the six parameters. Other oxygen algorithm parameters are assigned fixed values. The fitting procedure and the editing of outlying data are identical to those described in the earlier conductivity section if one substitutes the oxygen model (Equation 8) for Equation 5 in equations 6 and 7.

6.5 Oxygen Calibration Processing

The oxygen fitting procedure follows steps similiar to conductivity beginning with a data preconditioning step using program OXEXTRCT. Program OXEXTRCT extracts the down profile oxygen current and temperature at pressure levels corresponding to the up bottle levels and records these in the file to be fit along with the oxygen saturation value. The program used to determine the CTD oxygen model parameters from the water sample oxygen is called OXFITMR. The oxygen fitting procedure is illustrated schematically for PC processing in Figure 6 as are the three files created by OXFITMR. These files contain the same type of information for the oxygen calibrations as those created by program CONCALD for conductivity calibration. The fitting parameters and a histogram of the distribution of residuals are given in the sacciill.HIS file. Those data excluded from the fitting are logged to the sacciill.REJ file while those included are logged to the sacciill.RES file. A detailed description of the oxygen fitting program with examples of data files can be found in an article by Millard in WHPO 91-1 (1991) and in Appendix 4.

7. Post-Processing of CTD Data

After acquiring the CTD data, the four post-processing steps performed on the CTD data are: editing, pressure averaging, calculation of calibrated data quantities and pressure centering, and data quality control. Normally these steps are carried out on just the down-profile. The editing step can take place immediately after data logging, as it does not depend on calibrating against water sample data which are normally not available until the next day. However, water sample data calibration steps of matching CTD data to the station water samples should be completed before post-processing steps beyond pressure averaging are performed.

The CTD data are logged as a time series which, after first difference editing for spurious data values, is converted to a uniform pressure series in two steps as detailed in sections 7.2 and 7.3. Initially the pressure averaged temperature, conductivity and oxygen sensor data are output in an uncalibrated form. The pressure centering step allows rapid recalculation of salinity and oxygen data so that iterative data transformations can be done quickly as more refined salinity and oxygen sensor calibrations become available.

At sea, the pressure and temperature are scaled with the pre-cruise laboratory calibrations. Post-cruise laboratory calibrations are also performed soon after the CTD's arrive back from a cruise. All CTD data processing is considered preliminary until the post-cruise laboratory calibrations are complete, including the *in-situ* calibrations of conductivity (salinity) and oxygen, since these require laboratory calibrations of pressure and temperature. When the pre-cruise and post-cruise calibrations differ, the calibration closest in time to the observations is generally chosen unless problems with standards have been identified. Therefore the *in-situ* calibration of both conductivity and oxygen is taken over those done in the laboratory. The recent addition of portable temperature modules to WHOI CTD's has been a great asset in sorting out temperature calibration shifts.

7.1 Data Editing

Editing is used to correct errors in the station bookkeeping information of the station header and to identify erroneous observations in the raw CTD data. The data editing involves performing a first difference check of the data, and then marking suspect data in quality bytes appended to each CTD observation. The editing task involves identifying and/or correcting erroneous CTD observations in multiple passes through the station data file. It is not necessary to correct flagged errors before pressure averaging as program PRSAVG3 replaces flagged observations.

The error identification uses a first difference edit technique involving comparing the previous and current value of each variable against a difference criterion which can vary with variable and pressure. The edit program flags questionable observations on the error identification pass by setting data quality bytes appended at the end of each observation. The quality bytes identify erroneous variables within an observation in the following way. When a variable within a scan fails the edit criterion, a bit is set on in the quality bytes corresponding to the variable location within the scan. Details of the quality bytes implementation for CTD78 format can be found in the report by Millard et al. (1978). A similiar technique is used to flag error in the EG&G format.

The quality bytes identify several data conditions:

acquisition frame syncronization error,

first differences exceed edit criteria, interpolated data scans.

In a second editing step, observations flagged as erroneous can be corrected by linear interpolation.

7.2 Sensor Response Correction

Before converting raw CTD time series data to a pressure averaged data file, the sensor lag between temperature and conductivity data must be established. This must be carried out each time a new temperature sensor is installed. The response time of the Rosemount model 171 platinum temperature sensor relative to the 3-cm conductivity sensor used on the EG&G Mark IIIb CTD has been found by Millard (1982) to vary from 0.10 to 0.45 seconds. Because of this variation in the platinum temperature time constant, the fast thermistor has been removed from all WHOI Mark IIIb CTD's as discussed by Millard et al. (1980). Depending on the lowering rate, typically 1.0 to 2.0 m/s, the conductivity sensor has a flushing length response time of 0.015 to 0.03 seconds. The temperature/conductivity lag is determined empirically by adjusting the temperature lag so as to minimize salinity spiking as discussed by Fofonoff et al. (1974). Calculating the covariance and coherence phase between conductivity and temperature have also been used to estimate the temperature lag. We hope to replace these methods for establishing the temperature/conductivity time response in the near future with a technique using a laboratory dynamic response facility. This new apparatus is currently under development at WHOI by N. L. Brown.

To match the conductivity data time response to that of the temperature data, an exponential recursive filter is applied to conductivity sensor data (Millard, 1982). The equation used is

$$C(t) = C(t - \delta t) \cdot W_0 + C_i(t) \cdot W_1 \tag{9}$$

 C_i is the input conductivity, C is the output lagged conductivity, with

$$W_0 = e^{-\delta t/\tau}$$

$$W_1 = 1 - W_0$$

where τ is the platinum thermometer time constant, and δt is the time between CTD observations. The temperature probe time constant τ is stored as part of the instrument

calibration file. The pressure data are lagged with the same recursive filter yielding an internally consistent data set.

7.3 Creating a Uniform Pressure CTD Profile

The edited raw CTD data are gridded to form a centered uniform pressure series with calibrated salinity and oxygen data in two steps. The pressure averaging step replaces erroneous input data, applies the conductivity-temperature sensor lags, and bin-averages the raw data in uniform pressure steps (normally 2 decibars) resulting in a much reduced data series. Note that only pressure is output in engineering units. Because the CTD descent rate varies and data values are not uniformly distributed in pressure within each bin, the resulting averaged pressure series is not uniformly incremented in pressure. A pressure centering program is subsequently run to interpolate calculated temperature, salinity, oxygen and other engineering unit parameters to a uniform pressure grid. Both of these pressure averaged data files are stored as ASCII on the PC. The pressure averaging and centering steps are combined on the VAX and the output is stored as single precision real values in CTDVAX format (see Millard and Galbraith, 1982). Salinity is computed using the 1978 Practical Salinity Scale (PSS-78) (see Perkins and Lewis, 1980 and Fofonoff and Millard, 1983), and oxygen follows the algorithm of Owens and Millard (1985). By performing the salinity and oxygen calculations on the pressure averaged data, the number of these polynomial evaluations is significantly reduced (roughly by a factor of 50 for a 2 dbar averaging interval).

7.3.1 Pressure Averaging

The pressure average of temperature, conductivity, pressure and other parameters is performed in the time interval of observations occurring between the starting pressure P_0 and $P_0 + \delta P$. Owing to the variation in lowering rate, the output file is no longer a uniform time series, thus the time lag corrections, particularly between temperature and conductivity, must be carried out prior to the pressure averaging.

This section makes use of the following definitions:

 δt is the CTD instrument sampling interval (0.032 sec for a standard Mark IIIb)

 δP is the pressure averaging interval and the output pressure sampling interval.

jth refers to the jth pressure interval

 P_0 is the starting pressure of the interval

m is the number of observations averaged in the pressure interval.

The time averaged pressure $P(t - \frac{1}{2} m \delta t)$ is computed for pressures between $P_0 < P(t) < (P_0 + \delta P)$ as follows:

$$P(t - \frac{1}{2} m\delta t) = \frac{1}{m\delta t} \sum_{i=0}^{m\delta t} P(t)\delta t = P_{j}.$$
 (10)

 P_j is the time averaged pressure position of the CTD sensors within the pressure interval $(P_0 \text{ to } P_0 + \delta P)$, associated with the center pressure $P_0 + \frac{1}{2}\delta P$.

Pressure is lagged before averaging in the same manner as conductivity (equation 9), utilizing the equation

$$P(t) = P(t - \delta t) \cdot W_0 + P_i(t) \cdot W_1 \tag{11}$$

where P_i is the input pressure, and P is the output lagged pressure.

Although the shift in amplitude and phase of the pressure signal is small from filtering, the resultant pressure is more smoothly varying and better behaved for differentiating to compute lowering rate to look for changes in direction of the CTD package. The lowering rate $\delta P/\delta t$ must also be positive for data to be included in the above time average. This screens out data occurring during instrument pressure reversals due to the ship heave and roll, when the CTD sensors are in the wake of the instrument package and lack of flushing of the conductivity cell makes these measurements unreliable. When reversals occur, the previous value is substituted in order to preserve the time sequence. The substitution of the previous value produces a slight bias when pressure reversals occur, but usually the pressure reversals are short and appear infrequently within a typical profile. Expressed in mathematical notation, the lowering rate constraint is

when
$$\delta P(k)/\delta t < 0$$
, then $P(k) = P(k-1)$, $T(k) = T(k-1)$, and $C(k) = C(k-1)$.

The temperature and conductivity are averaged over the pressure interval (δP) after applying the lowering rate constraint above. The temperature and conductivity averages

are T_j and c_j located at the time averaged instrument position P_j . Except for pressure, these averages are carried out on the raw uncalibrated observations:

$$P_{j} = \frac{1}{m\delta t} \sum_{P_{0}}^{P_{0} + \delta P} (P(t)) \delta t \text{ engineering units}$$
 (12)

$$T_{j} = T(P_{j}) = \frac{1}{m\delta t} \sum_{P_{0}}^{P_{0} + \delta P} T(P(t)) \delta t \text{ unscaled}$$
 (13)

$$C_j = C(P_j) = \frac{1}{m\delta t} \sum_{P_0}^{P_0 + \delta P} C(P(t)) \delta t \text{ unscaled}$$
 (14)

where

$$N_j = N(P_j) = m$$
 is the number of observations in the pressure bin of width δP . (15)

Oxygen current, oxygen temperature and other CTD measurements such as redundant temperature, nephelometer, transmissometer, and so forth are averaged in the same way as temperature and conductivity in equations 13 and 14. The number of observations in each pressure averaged interval is carried along as a crude time base $(m\delta t)$ for oxygen lag correction and also to allow lowering rate $\frac{dP}{dt} = \frac{\delta P}{m\delta t}$ to be calculated. The raw average data are written to a file together with the scaled pressure. The pressure average output file has a name of ssccvttt.PRR on the PC.

7.3.2 Pressure Centering

The pressure centering step converts the data to physical units by applying the calibration polynomials discussed earlier and interpolates the pressure averaged observations to a uniform pressure series. In general, this data conversion is not reversible back to the uncalibrated data. Data calibration refinements use the pressure averaged data as a starting point unless changes to the pressure calibration or the temperature-conductivity lag are required. Depending on whether the instrument spends more or less time above the center pressure value $P_0 + \frac{1}{2} \delta P$, the time averaged pressure will be above or below the center pressure value. Hence a pressure interpolation is required to adjust the weighted average of temperature, salinity, oxygen, etc. to the center pressure as shown in equations 16 and 17. The difference between mean pressure P and the center pressure of the interval $P_0 + \frac{1}{2}\delta P$ is used together with the local temperature and the salinity gradients to adjust these properties to the center of the interval. The interpolation uses the average values from the adjacent pressure intervals to estimate these gradients.

Salinity is computed from the averaged values of pressure, temperature and conductivity before these observations are interpolated to the center pressure. Before computing salinity, the scaled conductivity is adjusted for conductivity cell deformations with temperature (α) and pressure (β) following Fofonoff et al. (1974) as shown in equation 2. An interpolation to the center pressure of each interval is required, because the temperature and conductivity averages T_j and C_j are located at the time averaged position within P_j which is not necessarily the center of the pressure interval beginning at P_i and centered at $P_i + \frac{1}{2} \delta P$. The gradients of temperature, salinity and oxygen are estimated from neighboring pressure intervals as follows:

For Temperature

$$T_{j}(P_{i} + \frac{1}{2} \delta P) = T(P_{j}) + [T(P_{j-1}) - T(P_{j+1})] \frac{(P_{0} + \frac{1}{2} \delta P - P_{j})}{(P_{j-1} - P_{j+1})}, \tag{16}$$

For Salinity

$$S_{j}(P_{i} + \frac{1}{2} \delta P) = S(P_{j}) + [S(P_{j-1}) - S(P_{j+1})] \frac{(P_{0} + \frac{1}{2} \delta P - P_{j})}{(P_{j-1} - P_{j+1})}.$$
 (17)

The oxygen sensor requires lag correction as described by Owens and Millard (1985). This lag correction of the oxygen current is done after the pressure averaging using the time information stored in the number of observations N_j as follows:

Oc =oxygen current with lag correction,

 Oc_i = measured oxygen current,

 τ_o = oxygen sensor lag of approximately 5-8 seconds,

$$Oc = Oc_j + \tau_o(\frac{\delta Oc}{\delta t}),$$

and the derivative of oxygen current is estimated as

$$\frac{\delta Oc}{\delta t} = [Oc_{j-1} - Oc_{j+1}] / (\frac{1}{2} [N_{j-1} + N_{j+1}] + N_j).$$
 (18)

It should be noted that adding the derivative of oxygen current with τ larger than unity causes resultant oxygen values to have a somewhat higher noise level. Lag corrected

oxygens are smoothed over 10 to 15 dbars. Oxygen is computed from oxygen current as given in equation 8.

7.4 CTD Data Processing Flow

A typical down-profile CTD station of 5000 decibars (1 hour) uses between 1.0 and 1.5 megabytes of storage on the μ VAX or the PC. Figure 7 illustrates the CTD data processing steps from the CTD instrument telemetry to a uniform pressure data file for the PC-based processing system. After recording the CTD data with CTDACQ, Figure 7 indicates that first difference editing is performed on the binary CTD data using the EG&G program CTDPOST. The edited CTD binary data file is compressed by pressure averaging with program PRSAVG3 to produce an ASCII output file that is only 2 percent of the input raw binary data file size. The pressure averaged data is then converted to uniform pressure intervals (PCENTER) with all variables converted to engineering units and salinity/oxygen computed. The CTD data processing steps used on the PC, with input and output files indicated, can be found in Appendix 3.

7.5 Data Quality Control

After the CTD station data is processed to a calibrated uniform pressure series, checks of the integrity of the calibrations and data editing are performed as follows. Temperature, salinity, oxygen and potential density anomaly profiles versus pressure are examined. A further data edit may be performed on the uniform pressure data file as required. The CTD calibration of salinity and oxygen are checked against the water sample data as follows. The CTD salinity and oxygen for a series of consecutive stations (typically four) is plotted versus potential temperature in the deeper region of the water column where salinity and oxygen variations are more predictable. The internal consistency of the CTD temperature, salinity and oxygen data is checked against an average CTD profile typically constructed by averaging together a group of neighboring stations on common pressure levels. A scaled value of the standard deviation, default is 3.8, of the average profile is used as a screening criterion with observations outside of this limit reported for further scrutiny. It is sometimes difficult to determine how closely the CTD should be expected to follow variations in the water sample data within a station as the water sample salinity and oxygen data both have uncertainties from sample to sample which are normally large compared to the station to station drift of the CTD. High quality water sample salinities have a repeatability (defined as one standard deviation) of $S = \pm 0.0018$ psu while oxygen is $O_2 = \pm 0.039$ ml/l according to Knapp and Stalcup (1987).

7.6 Comparison of PC and VAX Post-Processing Steps

Most of the basic data processing programs are identical on the MS-DOS PC's and VAX/VMS systems. Most of the CTD calibration and water sample processing programs are written in FORTRAN and run without modification on either system. The CTD pressure centering program is also implemented identically on both systems. However, the data logging programs are different as are the initial data storage formats adopted for the uncalibrated binary CTD data output. The VAX data logging program has adopted CTD78 (Millard et al., 1978) as an output format while the PC uses a binary format as documented in the EG&G software manual. The CTD pressure averaging program has identical processing and output section code but has been adapted to the different binary formats of the PC and μ VAX data acquisition systems. The initial water sample data files created by each acquisition program also have different formats. The water sample processing steps on both the VAX and PC systems put the water sample files into identical formats before the final water sample oxygen and salinity CTD parameter calibration steps. Some programs are only available on one computer system or the other. The transcribing programs which reformat data between machines are computer specific. Programs written in Quick Basic [QB on flow diagrams] are specific to the PC system.

8. Summary

The CTD data processing system described in this report is currently being used to process CTD data collected at WHOI. The report discusses editing and calibration steps that are required to insure the high quality CTD data. These include regular calibrations of CTD sensors against certified standards before and after a cruise and collection and calibration against high quality water sample salinities and oxygens to achieve an accuracy suitable for describing the deep ocean hydrography.

Areas of future enhancement to the post-processing system include: establishing the temperature and conductivity sensor lags using a laboratory dynamic calibration facility; adoption of the Benson and Krause (1984) oxygen saturation algorithm so as to conform to JPOTS recommendations; and the adoption of the VAX ship-cruise subdirectory oriented file naming convention on the PC which would eliminate this point of departure between the two systems and would allow the PC to include the cast number as part of the file name. An interactive menu program is being developed to integrate the various CTD post-acquisition processing steps (programs) together. We are exploring several approaches including event programming and dialog boxes to achieve a flexible and easy to use CTD processing system.

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Appendix 1: Brief Program Descriptions

This set of brief program descriptions is intended as an aid for following the series of CTD data processing flow diagrams. Following the program name the letters QB indicate programs written in Quick Basic. All other programs are written in FORTRAN.

CTD PC and VAX Computer Programs

Data Acquisition

CTDACQ QB

Purpose: To record raw CTD observations in EG&G format to mass storage (disk) and provide monitoring and data quality control plot and listing. The program also creates a file of CTD observations at water samples locations.

Data Editing

CTDPOST QB

Purpose: A first difference data editor to identify and examine erroneous CTD observations and mark for replacement during pressure averaging. Program also allows plotting and listing of data. Correction of EG&G header and calibration file information is presently accomplished with a text editor.

Calibration

LABCAL1

Purpose: The LABCAL1 program evaluates the polynomial coefficients relating the CTD pressure, temperature, and conductivity sensor observations to laboratory standard values. Polynomials up to third order can be evaluated for each sensor which are then employed in producing final calibrated CTD data.

PBIAS

Purpose: To create a file of pressure bias for the various stations of a cruise. This is a preparatory step before running CONVERT when a stainless steel pressure sensor is used.

CONVERT PC/VAX

Purpose: To invert salinity water sample to conductivity using the SAL78 FOR-TRAN algorithm described by Fofonoff and Millard (1983), to compute the difference between water conductivity and CTD conductivity, and to mark data quality. This is

a data preparation step before determining CTD conductivity parameters with program CONCALD.

CONCALD PC/VAX

Purpose: To fit for the CTD conductivity bias, slope and station dependent slope parameters as described by Fofonoff *et al.* (1974) and Millard (1982). CTD conductivity sensor data is fit to water sample salinity data that has first been inverted to conductivity (see program CONVERT above).

OXEXTRCT

Purpose: To extract raw temperature and oxygen sensor data from CTD downcasts at bottle trip levels and include with water sample oxygen. This is a data preparation step before determining oxygen algorithm parameters with OXFITMR.

OXFITMR PC/VAX

Purpose: To fit for the CTD oxygen algorithm parameters as described by Owens and Millard (1985). CTD oxygen sensor variables are fit to water sample oxygen data to determine up to 6 parameters of the oxygen algorithm. An edit is also performed on the input oxygen data to exclude bad observations from the calibration determination.

Creating Uniform Pressure CTD data

PRSAVG3

Purpose: Pressure Average converts the raw time series data in EG&G format from the CTD to a pressure averaged series. Time lags between sensors are corrected before pressure averaging and the sensor calibrations are applied to convert pressure data to engineering units before pressure averaging. All other variables are averaged and reported unscaled. The conversion of measured variables to salinity or oxygen and the adjustment of data to uniform pressure intervals is left to a separate program, PCENTER, to facilitate data recalibration. Calculated data are goored in an output file in ASCII.

PCENTER

Purpose: To convert the raw pressure average data to a centered uniform pressure averaged series with salinity and oxygen replacing conductivity and oxygen sensor measurements, to interpolate across gaps in pressure, and to update the header minimum and maximum data values. The calibration data are applied to raw data except pressure.

Format Conversion

PCTDVAX VAX

Purpose: PCTDVAX converts EG&G PC format pressure averaged ASCII data files to CTDVAX format Millard and Galbraith, 1982. The program unpacks ASCII header records at the beginning of input file and stores the information in CTDVAX header record. Data scans are translated to VAX single precision values and pressure becomes implicit with only the minimum pressure and increment stored.

VAXTONB PC and VAX

Purpose: VAXTONB converts NODCEXCH format VAX pressure averaged ASCII data files to same uniform pressure ASCII file format as PC program PCENTER (see Appendix 3). This program allows CTD data stored on the VAX to be used on the PC.

Data Quality Control

BTLEXTR

Purpose: To reformat water sample data file created by CTDACQ Version 3 to include only unscaled data from raw binary CTD data file and record numbers from CT-DACQ bottle and __.EDT files.

WOCETMPL

Purpose: Program WOCETMPL reads the unscaled averaged CTD observations recorded at bottle trips. The program scales the data to physical units including a weighted down/up pressure hysteresis correction used for stainless steel pressure transducers. The data is put into a standard WOCE format template with water sample data place savers set to -9. Any corrections to the bottle numbers or their order must be done before water sample data can be merged into the file using MERGE_SO.

MERGE QB PC

Purpose: Program MERGE reads the template file created by WOCETMPL and merges in Salts and Oxygens from the hydrographic data base on a station by station basis. The program will also merge other water sample data such as CFC's or nutrients. The data is merged by bottle number in the template file.

BTLMRG

Purpose: Program BTLMRG merges the water sample salinity and oxygen values from the WOCE water sample file supplied by the hydrographic group with the raw CTD data stored in the _____.BT2 file of program BTLEXTR. The data is merged cross-

referencing the raw pressure and the bottle number of the hydro group is file. The output file when concatenated with other ______.BT2 files becomes input to CONVERT, one of two steps in determining conductivity calibrations.

OXUPDATE

Purpose: Program OXUPDATE merges the uncalibrated down profile oxygen sensor data with the up-profile uncalibrated CTD data in the ___S___.BT2 file. The output ___S___.BT3 file is then reprocessed through WOCETMPL with a modified calibration file to produce calibrated CTD oxygen and salinity data in the WOCE water sample format. OXUPDATE is not necessary for water samples collected on the down profile or for oxygen sensor data exhibiting no down/up profile hysteresis.

10DBAVER QB

Purpose: to average 2 decibar CTD data to 10 decibar intervals for both archiving and plotting with bottle data.

NBTOGR QB

Purpose: To compute potential temperature and potential density anomaly from 10 decibar CTD data file for overplotting with bottle data.

HDRFMT QB

Purpose: To produce a summary listing of station header (bookkeeping) information over the cruise, including position, date, time and depth.

CTDAVG1

Purpose: To create an average profile of a group of stations on pressure horizons. The mean values and standard deviation of temperature, salinity and oxygen arc written to an ASCII file together with the number of observations included in the averaging and the stability parameter.

CTDEDT

Purpose: To compare individual profiles to a mean profile created by CTDAVG1 and identify levels failing an edit criterion involving the standard deviation of temperature, salinity and oxygen from the mean profile scaled by a multiplicative factor.

CTDLIST

Purpose: To create a summary of physical properties of sea water at standard or selected pressure levels. The standard-levels listing has a single page format for cruise reports.

Appendix 2: File Naming Conventions

1. File name format for files used in laboratory calibrations:

PC and VAX file name format:

iivmmmyy.ext

where

```
ii = instrument number (2 chars)
v = variable letter code (1 char P, T, or C)
mmm = month (3 chars)
yy = yea. (2 chars)
```

example: 10PJUN93.CAL 2. PC and VAX file extensions:

CAL source calibration file,

FIT polynomial regression coefficients

and residuals, or

DIF differences between instrument observations and standards.

Filename format for files used for individual profiles (stations):

Filename format for PCs:

ssccvttt.ext

where

ss = ship designation (2 chars)
cc = cruise number (2 chars)
v = version letter code (1 char U, D, S)
ttt = station number (3 chars)

example: KN38D001.EDT

Filename format for VAXes:

ttttvppp.ext

where

tttt = station number (4 chars)
v = version number (1 char)
ppp = cast (profile) number (3 chars)

example: 0001A001.EDT

(Sub)directory name format for VAXes:

sscccvnnn

where

ss = ship designation (2 chars)
ccc = cruise number (3 chars)
v = version letter code (1 char)
nnn = project number designation (3 chars)

example: KN138P003

NOTE: The examples in the text generally use the PC formats, not the VAX formats.

VAX use of file extensions:

CTD	CTDVAX format pressure data file
DYN	Georgi format water sample file
EDT	AQUI89 edited CTD78 data file
ERR	AQUI89 error file
HED	AQUI89 ASCii header/calibration file
LOG	AQUI89 journal file
RAW	AQUI89 raw CTD78 data file
WSC	AQUI89 scaled water sample file
WRW	AOUI89 unscaled water sample file

PC use of file extensions:

COO CTDACQ calibration file
HDR CTDACQ header file
EDT Edited unscaled binary data file
PRR pressure averaged data file (ASCII)
PRS pressure centered data file (ASCII)
RAW CTDACQ unscaled binary data file

NOTE: Files whose file extensions are SAL and OX are named according to conventions established by the hydrographic group and therefore do not follow the file naming conventions described in this report.

PC and VAX filename format:

sscciill.ext

where

ss = ship designation cc = cruise number ii = instrument number ll = cruise leg designation

and

BT2 Reformatted unscaled water sample file with water sample salinity/oxygen BT3 format of BT2 file but down oxygen data BLT CTDACQ water sample file C00 CTDACQ calibration file CFC WOCE water sample format freon data file CTP WOCE water sample format recalibrated file HIS Salt/Oxygen fit parameter/histogram file RES Salt/Oxygen fitting residual file LST merged unscaled water sample data file LOG Program journal files NUT WOCE water sample format nutrient file REJ Salt/Oxygen fitting rejects file SEA WOCE water sample format merged file used to develop CTD calibrations. SOX WOCE water sample format Hydrography file TMP WOCE water sample format template file

Appendix 3: CTD Processing Flow

The following lists the CTD and water sample processing steps (programs) and data files associated with data processing on PC computers. The CTD conductivity and oxygen calibration and conversion to uniform pressure CTD data file are seldom done only once. The processing order outlined is typical but not necessarily the only order that may be followed. This Appendix will change as programs evolve; it is maintained in a documentation file together with the program documentation files and programs.

1. Acquire the data using the EG&G software package

CTDACQ input IM##SSCC.C00 with pre-cruise laboratory

calibrations for that instrument

output ssccDttt.RAW raw downcast CTD data file ssccUttt.RAW raw upcast CTD data file

(note: these raw files are read only and need attributes

changed in order to delete them.)

ssccDttt.EDT raw downcast CTD data file ssccUttt.EDT raw upcast CTD data file

ssccDttt.HDR header station identification file

sscc Uttt.BTL rosette water sample file sscc Dttt.C00 calibration file for that station (note: it is necessary to copy *D*.C00 to *U*.C00 so there is a calibration file for

processing rosette data as well

(This file is read only.)

2. Edit the data using the EG&G software package

CTDPOST input ssccvttt.C00 file with correct laboratory calibrations for

that station

ssccvttt.HDR header file for that station

ssccvttt.EDT binary data file

output ssccvttt.EDT edited binary data file:

input file overwritten

3. Scale the raw CTD data with laboratory pressure calibrations and correct temperature lag and scan rate. It is important to have these three things correct at this point. The default averaging interval is two decibars. The output of this step is the starting point for calibration refinements. Data are compressed to about 2 decibars in an ASCII form. Data output is not converted to engineering units except for pressure. Data flagged as erroneous in the ssccvttt.EDT file are not included in pressure averaged output file.

PRSAVG3 input

ssccvttt.C00 file with correct laboratory calibration

ssccvttt.EDT edited raw data file

ssccvttt.HDR

output ssccvttt.PRR

4. This is the salt and oxygen calibration loop! Data are scaled with best calibrations. This step is repeated as necessary in order to apply refined temperature, conductivity, and oxygen calibrations with updated *.C00 files.

PCENTER input

ssccvttt.PRR

ssccvttt.HDR

ssccvttt.C00

output ssccvttt.PRS scaled 2 decibar data

5. Data are listed at selected levels for presentation to the Principal Investigator.

CTDLIST input

ssccvttt.PRS

PSTAR.DAT (optional PRESSURE LEVELS)

(edit this to include desired PR levels)

output

ssccvttt.LTG

output ssccvttt.DAT

WATER SAMPLE PROCESSING (of upcast data)

1. Rosette data file is reformatted to contain all uncalibrated CTD parameters needed to calculate CTD pressure, temperature, salinity and oxygen. Blank columns are output for the eventual input of rosette salinity and oxygen values. Program gets scan number from ssccvttt.BTL file and extracts an average of 10 scans (default) from the ssccvttt.EDT file to match.

BTLEXTR input

sscc Uttt.BTL upcast rosette file from acquisition

sscc Uttt. EDT upcast ctd file from acquisition

output sscc Uttt.BT2 unscaled CTD rosette file

2. The unscaled rosette file is scaled with the best calibration file available. A WOCE template water sample file is created for distribution to various water sampling groups for data input. Care must be taken to insure the integrity of the bottle number order as the water sample data are entered.

WOCETMPVL input TEMPLATE.HDR This is a template file specific

to the cruise. If it does not exist in the working directory, then the program will create it.

ssccvttt.BT2 unscaled CTD rosette file ssccvttt.C00 most recent calibration file

output ssccvttt.TMP scaled ASCII rosette file

3. At this point the hydrographic group merges the rosette water sample salts and oxygens into the sscc Uttt. TMP file and passes back a sscc Uttt. SOX file to the CTD data processor. The hydrographers plot theta/S and theta/O2 and reorder the bottles if required.

MERGE input _____.SAL input file from salinometer _____.OXY input file from oxygen titration

input sscc Uttt.SOX

Q1EDIT output ssccUttt.SOX

This program plots theta/S, theta/O2. It allows changing flags on SA + OX. If the order of bottles needs to be changed, it will show up here. The order can be changed manually by editing the *.TMP file and then remerging and plotting.

4. Rosette water sample salts and oxygens are merged back in with the unscaled CTD scans based on bottle number and pressure.

BTLMRG input sscc Uttt.SOX WOCE template with salts and oxygens

sscc Uttt.BT2 unscaled CTD rosette file without SA & OX

output sscc Uttt.BT2 unscaled CTD rosette file without SA & OX

ssccvttt.BT2 for each station

ssccvttt.C00 one calibration file with the laboratory calibration being used for the cruise.

CONDUCTIVITY FITTING PROCEDURE

1. The first step is to run PBIAS: The input to this program is the ssccvttt.c00 file for each station. You can run a group of stations using the batch mode (i.e. a ssccv.dir file). To create a batch input file, type "dir ssccD*.c00>sscc.dir" at the DOS prompt, then when you run PBIAS enter this file name at the prompt.

2. The next step is to run CONVERT; this program requires the following files as input: ssccv.LST (a group of ssccvttt.BT2 files appended together, with header). The header need only be ENDHDR in the first 6 positions of this line immediately preceding the data. Any number of lines of text describing the calibration data, etc. can be inserted prior.

ssccv.C00 a copy of one of the original down calibration files from the station group

ssccv.C0U a copy of one of the original up calibration files from the station group only for stainless steel transducer**

ssccv.PBI from PBIAS**.

** not neede calibration file contains Pressure Temperature — variable 14 (i.e. only for stainless steel transducer)

The output from CONVERT is:

ssccv.WSD; the CTD data converted to engineering units with nominal conductivity.

3. Run CONCALD, the input to this program is the output from CONVERT. The input file must have the extension ssccv.WSD.

You can designate different groups by copying and editing this file into the appropriate groups for fitting (the header must always be present).

Follow the documentation for this program as it explains how to answer the prompts. You can also default your way through the prompts. Select 1/ to obtain a bias and slope.

Three files are output:

ssccv.HIS histogram of residuals

with calculated conductivity coefficients

ssccv.REJ rejected observations whose residuals exceed edit factor times

standard deviation

ssccv.RES final observations and residuals not rejected

OXYGEN FITTING PROCEDURE

1. The first step is to run OXEXTRCT, this program requires the following as input: ssccv.LST (same input to CONVERT),

sscc (Ship and Cruise number).

Use / to use the default *.c00 calibration file)

ssccvttt.HDR
ssccvttt.C00
ssccvttt.PRR

one for each station must be present in data directory

The program outputs a file *.oxy which is used as input to the next step, OXFITRM:

ssccv.OXY

2. Run OXFITMR, the input file must have extension *.oxy:

ssccv.OXY

You can make up groups of stations by copying and editing your output from ssccv.oxy. The header must always come first for all fitting groups. You can default through the prompts to obtain three output files:

ssccv.HIS histogram of watersample-ctd residuals

with calculated oxygen coefficients

ssccv.REJ rejected observations

ssccv.RES final observations and residuals

The documentation for OXEXTRCT and OXFITMR will give you more information on run time parameters.

FINAL PROCESSING

- 1. Once the data have been fitted to refine conductivity calibrations, then
 - a. Updated unscaled water sample data files are produced with the down-profile oxygen measurements using program OXUPDATE.

input ssccSttt.BT2

sscc.OXY contains down Oc and Ot from OXEXTRCT

ssccSttt.C00 calibration file

output ssccSttt.BT3 this has the down oxygen

measurements merged

- b. The ssccDttt.C00, ssccSttt.c00 and ssccUttt.C00 files should be edited to reflect any calibration changes.
- c. New WOCE format water sample data files are created using program WOCE-TMPL.

```
input ssccSttt.BT2 or ssccSttt.BT3
ssccSttt.C00 with refined calibration
output ssccSttt.CTP this has the best pressure, temperature, salinity values;
oxygen refinements to be done later
```

- d. New CTD data files can be created using program PCENTER inputting the updated ssccDttt.C00 files with refined calibrations.
- e. New station listings can be created using program CTDLIST using files created in step d above as input.

It is a good idea at the end of processing a station to separate all the output files of various steps into individual directories named to indicate the data form contained. This helps to keep down the clutter.

COPYALL.BAT

```
copy *.prr \ctdata\prr\*.*
copy *.prs \ctdata\prs\*.*
copy *.ltg \ctdata\lst\*.*
copy *.tmp \ctdata\tmp\*.*
copy *.bt2 \ctdata\bt2\*.*
```

DELEALL.BAT

del *.prr

del *.prs

del *.ltg

del *.tmp

del *.bt2

Appendix 4: Details of Conductivity and Oxygen Fitting Procedures

GENERAL

This section is intended as a users' guide for fitting CTD conductivity (salinity) and oxygen variables to water sample salts and oxygens. There are no hard and fast rules for deciding the best calibrations for a data set as the calibration of the data set from each cruise provides its own set of challenges. There are three output files from both CONCALD (conductivity fitting program) and OXFITMR (oxygen fitting program) used to evaluate the quality of the fits to the data and resultant calibrations.

The three files produced by both the conductivity and oxygen fitting programs to evaluate the calibrations of a group of stations are histogram, residuals, and rejects. The evaluations of the conductivity and oxygen fits involve looking at the residuals defined as difference of the water sample minus the CTD conductivity. The residuals of the final fit are contained in a file named ssccv. RES. A file containing a histogram of the residuals from the final fit and calibration coefficients has an extension of ssccv. HIS. A third file contains the observations excluded from the final conductivity or oxygen fit and has an extension of ssccv. REJ. The data rejected from the fit are looked at during the cruise to see if a common pattern, such as a leaky bottle, is the cause of the data being excluded. The residuals of the final fit stored in the ssccv.RES file are plotted against station number and pressure to determine the quality of the calibrations. It is very important to keep in mind when looking at the residuals from either the conductivity or oxygen fitting that the residuals are a difference and when residuals from a station or a group of stations residuals depart from the zero line that it indicates that either the CTD or the Water Sample data are questionable. Since the conductivity and oxygen fitting programs use the same extensions, they are distinguished by keeping files for each sensor in a separate data directory (recommended) or by giving them different file names (also helpful).

Grouping the station data is very important to fitting both conductivity and oxygen data. It is desirable to fit over the largest possible group of stations of a particular instrument (the entire cruise) provided sensors haven't been changed. The assumption is that the CTD sensors are stable and that fitting over a group of stations reduces the uncertainty of the water sample data variability. The validity of this assumption is tested by plotting the residuals of the fit versus station number. It is very important to note changes to the instrument's configuration (i.e. replacement of the oxygen or other sensors) including the opening of the instrument. Swapping out of an instrument or a sensor replacement normally requires starting a new calibration group.

During a cruise, calibration groupings are continually being extended as more water sample data are collected and analyzed. Both the oxygen and conductivity sensors' calibrations have been observed to change more rapidly at the beginning of use during a cruise, so waiting 10 to 12 stations before settling on preliminary calibrations for both sensors is a good idea.

CONDUCTIVITY

The NBIS EG&G Mark IIIb conductivity-temperature-depth (CTD) device employs a 3 cm long four electrode alumina conductivity sensor made by the manufacturer. Over the course of a cruise, the conductivity sensor has been observed to drift 0.010 mmho/cm per month. This is beyond the accuracy requirements necessary to describe deep water salinity variations (Millard, 1982). Therefore, continual monitoring and recalibration of the conductivity sensor against water sample salinity data is necessary to obtain the highest quality results necessary.

The water sample data are currently analyzed on a Guildline model 8400 salinometer calibrated against standard water before and after running each batch of samples (typically encompassing data from three or four stations). The CTD salinity is computed on the Practical Salinity Scale of 1978 using a FORTRAN algorithm SAL78(C,T,P,0), where conductivity (C), temperature (T) and pressure (P) are as as discussed earlier in sections 4.6 and 6.2. Therefore an error in CTD salinity of 0.001 psu can result from an error in conductivity of 0.001 mmho/cm, temperature of 0.001 C, or pressure of 2.5 dbars. So a CTD salinity shift of 0.005 psu, although most likely resulting from a conductivity shift of 0.005 mmho/cm, might also result from a temperature shift of 0.005 C or pressure offset of 12 decibars.

The conductivity calibration program CONCALD provides several methods of establishing calibration parameters. The laboratory calibration often provides good conductivity slope adjustment and bias parameters. The conductivity bias obtained from using the variable salinity baths at room temperature has proved particularly reliable. For this case, fitting for a conductivity slope is all that is normally required. This fit can be performed to either all pressure levels or just data from the deep water (P > 2000 decibars). Fitting to the deep water eliminates regions that have strong vertical gradients of salinity that will bias the conductivity slope if there is a vertical separation (or time separation with ship's heave) between the rosette bottles and CTD sensors (the rosette is typically 1.5 meters above the CTD). Because of stronger vertical salinity gradients in the shallow layer, final conductivity calibrations are normally established to the deep (p > 2000 dbars) levels. When the conductivity bias is found using the water sample data, a two-part conductivity fitting procedure is adopted. First conductivity bias and slope are derived from water sample data at all levels, since this provides a larger range of conductivity (60 to 32 mmho/cm) over which to determine both bias and slope. The bias is then input to refit the deeper levels' data (p > 2000 dbars) to redetermine the conductivity slope. Besides fitting the conductivity slope alone and bias and slope, a linear station-dependent conductivity slope can be found with or without conductivity bias determination.

Examples of Conductivity Data Evaluation

The CONCALD program was run on the ssccv. WSD file for stations 74 through 80 of Hesperides Cruise 6.

The following is a partial list of the input data used to produce the calibrations that follow: Note that the ssccv.WSD file pressure and temperature are the best calibrated CTD values while the CTD conductivity is nominally scaled to engineering units (slope = 0.001) and corrected for materials deformation effects (see section 4.6). The water sample conductivity is obtained by inverting the water sample salinity with the CTD temperature and pressure as discussed in section 6.2. The conductivity difference column 7 C(WS-CTD) uses the calibration file conductivity calibration (i.e. column 7 = column 6 - $[E_2 + D_2 \cdot G_r]$ where G_r is column 5 times 1000). See section 4.6 titled "Conversion to Engineering Units" for further details. If the calibration file contains the correct conductivity calibrations, then the average of the conductivity differences in column 7 will be zero.

TYPE HE06-74.WSD

Sta.	Fir.	Press	${\tt Temp}$.	C(ctd)	Cond(WS)	C(WS-CTD)	Salt(WS)	Oxy(WS)	Qual.
====	=====	======	*******		=======			=======================================	=====
74	1	5905.6	2.0540	32.9186	32.9249	0.00300	34.8430	5.6880	0
74	2	5499.0	2.0139	32.7634	32.7701	0.00334	34.8460	5.7080	0
74	3	4995.6	2.0962	32.6937	32.7007	0.00331	34.8653	5.8350	0
74	4	4500.6	2.2657	32.7038	32.7105	0.00271	34.8928	6.0460	0
74	5	4000.5	2.3183	32.5856	32.5918	0.00211	34.8989	6.0050	0
74	6	3500.4	2.4813	32.5636	32.5704	0.00238	34.9135	5.9510	0
74	7	3001.1	2.7562	32.6403	32.6478	0.00281	34.9361	5.8500	0
74	8	2501.4	3.1011	32.7782	32.7861	0.00280	34.9647	5.8450	0
74	9	1877.5	3.8715	33.2663	33.2739	0.00175	35.0238	5.7350	0
74	10	1497.0	4.5465	33.7342	33.7428	0.00223	35.0467	5.7690	0
74	11	998.7	6.6552	35.4426	35.4462	-0.00448	35.0407	3.9040	0
74	12	802.0	9.4074	38.1385	38.1800	0.03114	35.3060	3.5780	0
74	13	600.8	13.3025	42.3605	42.3439	-0.03062	35.7786	4.1010	0
74	14	498.8	15.0179	44.2691	44.2872	0.00231	36.0347	3.8740	0
74	15	402.2	16.7475	46.3206	46.3210	-0.01720	36.3188	4.2020	0
74	16	301.4	17.9977	47.7737	47.7941	0.00144	36.5152	4.4400	0
74	17	249.2	18.4712	48.3244	48.3329	-0.01100	36.5737	4.4800	0
74	18	198.5	19.0584	48.9759	49.0042	0.00823	36.6404	4.4200	0
74	19	174.8	19.4439	49.4348	49.4529	-0.00246	36.6853	4.4240	0
74	20	151.3	20.0028	50.0892	50.1131	0.00271	36.7518	4.6060	0
74	21	122.9	20.8888	51.0994	51.1051	-0.01644	36.8035	4.5590	0
74	22	101.0	21.8288	52.1339	52.1398	-0.01726	36.8348	4.7670	0
74	23	51.1	24.3814	54.8280	54.7798	-0.07409	36.7623	5.1570	0
74	24	25.7	28.5146	59.3169	59.2749	-0.07264	36.7420	4.6480	0
75	1	5991.1	2.0648	32.9531	32.9583	0.00194	34.8417	5.6840	0
75	2	5607.0	2.0266	32.8064	32.8111	0.00130	34.8425	5.7070	0
75	3	5091.0	2.1035	32.7302	32.8172	0.08340	34.9607	5.8190	0

```
75
         4576.9
     4
                   2.2557
                            32.7178
                                      32.7212 -0.00045
                                                                     5.9960
                                                          34.8858
                                                                              0
75
     5
         4063.1
                   2.3219
                            32.6114
                                      32.6159
                                                0.00037
                                                          34.8980
                                                                     6.0470
                                                                               0
75
     6
         3552.1
                   2.4804
                            32.5818
                                      32.5867
                                                0.00054
                                                          34.9118
                                                                     5.9780
                                                                               0
75
     7
         3040.1
                   2.7393
                            32.6387
                                      32.6448
                                                0.00138
                                                          34.9329
                                                                     5.8470
                                                                               0
75
     8
         2532.9
                   3.0768
                            32.7691
                                      32.7755
                                                0.00132
                                                          34.9632
                                                                     5.7800
                                                                               0
75
         2022.1
     9
                   3.6465
                            33.1119
                                      33.1198
                                                0.00226
                                                          35.0103
                                                                     5.7940
                                                                               0
75
    10
         1767.5
                   4.0772
                            33.4178
                                      33.4265
                                                0.00266
                                                          35.0394
                                                                      5.7290
                                                                               0
75
    11
         1515.8
                   4.5173
                            33.7246
                                      33.7334
                                                0.00245
                                                          35.0572
                                                                     5.6260
                                                                               0
75
    12
         1336.7
                   5.0210
                            34.1244
                                      34.1328
                                                0.00164
                                                          35.0794
                                                                     5.3440
                                                                               0
75
         1159.8
                   5.6685
                            34.6399
    13
                                      34.6469 -0.00037
                                                          35.0800
                                                                      4.7920
                                                                               0
75
    14
         1012.0
                   6.5322
                            35.3485
                                      35.3581
                                                0.00165
                                                          35.0620
                                                                      4.0640
                                                                               0
                   7.9786
75
    15
          858.3
                            36.6645
                                      36.6786
                                                0.00492
                                                          35.1141
                                                                      3.3770
                                                                               0
                  10.1904
                            38.9292
75
    16
          731.3
                                      38.9530
                                                0.01277
                                                          35.3658
                                                                      3.4390
                                                                               0
75
    17
          604.5
                  12.8336
                            41.7627
                                      41.8028
                                                0.02658
                                                          35.7023
                                                                      3.9160
                                                                               0
75
    18
          478.1
                  15.2659
                            44.5570
                                      44.5875
                                                0.01449
                                                          36.0885
                                                                      4.3440
                                                                               0
75
    19
          351.9
                  17.3368
                            46.9887
                                      47.0052 -0.00165
                                                          36.4061
                                                                      4.4090
                                                                               0
75
    20
          252.4
                  18.3113
                            48.1377
                                      48.1517 -0.00525
                                                          36.5604
                                                                      4.5820
                                                                               0
75
    21
          175.9
                  19.0733
                            48.9854
                                      49.0095
                                                0.00392
                                                                      4.5910
                                                          36.6402
                                                                               0
    22
                                      50.9752 -0.01212
75
          101.3
                  20.7826
                            50.9652
                                                          36.7977
                                                                      4.9040
                                                                               0
75
    23
           51.2
                  23.5501
                            53.8037
                                      53.8173 -0.01134
                                                          36.7149
                                                                      5.2330
                                                                               0
75
    24
            9.9
                  28.4447
                            59.1737
                                      59.1927 -0.01147
                                                          36.7435
                                                                      4.5730
                                                                               0
         5856.3
76
     1
                   2.0475
                            32.8986
                                      32.9039
                                                0.00201
                                                          34.8422
                                                                      5.6910
                                                                               0
76
     2
         5498.1
                   2.0202
                            32.7692
                                      32.7737
                                                0.00109
                                                          34.8441
                                                                      5.7090
                                                                               0
76
                   2.1346
     3
         4994.2
                            32.7307
                                      32.7359
                                                0.00151
                                                          34.8678
                                                                      5.8540
                                                                               0
76
     4
         4491.3
                   2.2700
                            32.7050
                                      32.7100
                                                0.00105
                                                          34.8914
                                                                      6.0260
                                                                               0
76
     5
         4000.6
                                                          34.8991
                   2.3318
                            32.5982
                                      32.6039
                                                0.00158
                                                                               0
                                                                      5.9880
```

The following is a histogram of the final fit data and the associated conductivity calibration constants:

A) The histogram file below is fitting for both conductivity bias and slope for stations 74–80 at all pressure levels. Notice that at iteration 17 no further reject data were identified and that a histogram follows with a standard deviation of .0018 mmho/cm.

TYPE HE06-74 HIS

```
PC PROGRAM CONCALD DOUBLE PREC. May 11, 1990
  NUMBER OF DATA POINTS INPUT =
                                      167
STATIONS
             74.
                   80.
                        PRES. BOUNDS
                                             0.0
                                                   6500.0 edit=
                                                                  2.8
 APPLIED COND. BIAS 0.0000
PASS No. =
                        1
 PASS No. =
                       15
                           C,
     St.#,
            Р,
                   Τ,
                                  COEFF.
                                                      >G00D
      0.00
            0.00
                   0.00
                          0.00
                                 -.76375605E-02
                                                     7.53
```

```
0.00
           0.00
                  0.00 1.00
                                0.10004104E-02
                                                  0.387E+05
N =
       123 AVE=
                   -0.26573E-14 STD. DEV.=
                                                0.22727E-02
PASS No. =
                     16
                          C,
    St.#,
           Р,
                                 COEFF.
                                                    >G00D
    0.00
                        0.00
                                -.77806407E-02
           0.00
                  0.00
                                                   8.69
     0.00
           0.00
                  0.00
                        1.00
                                0.10004126E-02
                                                  0.437E+05
 N=
       120 AVE=
                    0.29014E-14 STD. DEV.=
                                                0.19998E-02
PASS No. =
                     17
    St.#,
           Ρ,
                  Τ,
                          С,
                                 COEFF.
                                                    >GOOD
  1 0.00
                  0.00
                       0.00
                                -.84434914E-02
           0.00
                                                   10.1
     0.00 0.00
                  0.00
                        1.00
                                0.10004328E-02
                                                  0.466E+05
 N=
       118 AVE=
                   -0.30710E-14 STD. DEV.=
                                                0.18394E-02
CLASS INT:
              0.002000
  -5
       0
  -4
       0
  -3
       0
  -2
   0
   1
   2
       3***
   3
       2**
   4
       0
   5
       0
   118
          AVERAGE =
                          0.000000
                                      ST. DEV. =
                                                      0.001839
```

B) The histogram file below is fitting for a station-dependent conductivity slope over stations 74-80 for the pressure levels greater than 1500 decibars. The edit criterion for rejecting residuals is 2.8 standard deviations, and those data excluded from the final fit are listed in the HE06-74A.REJ file which follows the histogram file listing. Notice that the standard deviation is reduced to 0.0011 mmho/cm primarily because the data above 1500 dbars are not included. A summary of station by station conductivity slope values is listed after the histogram.

TYPE HE06-74A.HIS

```
PC PROGRAM CONCALD DOUBLE PREC. May 11, 1990
 NUMBER OF DATA POINTS INPUT = 68
STATIONS 74. 80. PRES. BOUNDS 1500.0 6500.0 edit= 2.8
APPLIED COND. BIAS-0.0084
PASS No. =
    St.#, P, T, C, COEFF.
                                         >GCOD
  1 0.00 0.00 0.00 1.00 0.10024593E-02 704.
  2 1.00 0.00 0.00 1.00 -.25899925E-07 1.40
 N= 68 AVE= 0.14989E-06 STD. DEV.= 0.98020E-02
                 2
PASS No. =
   St.#, P, T, C, COEFF.
                                         >G00D
  1 0.00 0.00 0.00 1.00 0.10010267E-02 0.597E+04
  2 1.00 0.00 0.00 1.00 -.77520487E-08 3.56
 N= 67 AVE= -0.47673E-05 STD. DEV.= 0.11453E-02
 CLASS INT: 0.002000
  -5
  -4 0
  -3 0
  -2 0
   1 12********
   3 0
   4 0
   5 0
    67 AVERAGE = -0.000005 ST. DEV. = 0.001145
           COND. SLOPE
  STATION
      74. 0.10004530E-02
      75. 0.10004453E-02
      76. 0.10004375E-02
      77. 0.10004298E-02
      78. 0.10004220E-02
      79. 0.10004142E-02
      80. 0.10004065E-02
```

The following is a partial list of those data included in the final fit procedure for pressures greater than 1500 dbars. The residual column 7 is plotted versus station and pressure to see how well the CTD conductivity matches the water samples.

TYPE HE06-74.RES

#	Station	Prs.	Tmp.	Cctd	Cws	residual	[Cws-Cctd]
1	74.0	5905.6	2.0540	32.9102	32.9249	-0.00017	
2	74.0	5499.0	2.0139	32.7550	32.7701	0.00030	
3	74.0	4995.6	2.0962	32.6853	32.7007	0.00063	
4	74.0	4500.6	2.2657	32.6954	32.7105	0.00033	
5	74.0	4000.5	2.3183	32.5772	32.5918	-0.00012	
6	74.0	3500.4	2.4813	32.5552	32.5704	0.00049	
7	74.0	3001.1	2.7562	32.6319	32.6478	0.00116	
8	74.0	2501.4	3.1011	32.7698	32.7861	0.00150	
9	74.0	1877.5	3.8715	33.2579	33.2739	0.00097	
25	75.0	5991.1	2.0648	32.9447	32.9583	-0.00103	
26	75.0	5607.0	2.0266	32.7980	32.8111	-0.00146	
27	75.0	4576.9	2.2557	32.7094	32.7212	-0.00272	
28	75.0	4063.1	2.3219	32.6030	32.6159	-0.00158	
29	75.0	3552.1	2.4804	32.5734	32.5867	-0.00116	
30	75.0	3040.1	2.7393	32.6303	32.6448	0.00001	
31	75.0	2532.9	3.0768	32.7607	32.7755	0.00025	
32	75.0	2022.1	3.6465	33.1035	33.1198	0.00160	
33	75.0	1767.5	4.0772	33.4094	33.4265	0.00226	
34	75.0	1515.8	4.5173	33.7162	33.7334	0.00223	
35	76.0	5856.3	2.0475	32.8902	32.9039	-0.00065	
49	76.0	5498.1	2.0202	32.7608	32.7737	-0.00139	
50	76.0	4994.2	2.1346	32.7223	32.7359	-0.00068	
51	76.0	4491.3	2.2700	32.6966	32.7100	-0.00086	
52	76.0	4000.6	2.3318	32.5898	32.6039	-0.00012	
53	76.0	3500.2	2.5021	32.5749	32.5898	0.00069	
54	76.0	3002.0	2.7497	32.6272	32.6428	0.00137	
55	76.0	2498.5	3.0750	32.7454	32.7596	-0.00009	
56	76.0	2000.8	3.6599	33.1109	33.1260	0.00065	
57	76.0	1501.2	4.7369	33.9326	33.9478	0.00039	

The following is a list of those data excluded from the final fit procedure for pressures greater than 1500 dbars. This file is also reviewed by the hydrographic group since the water sample data is potentially erroneous.

TYPE HE06-74.REJ

#	Station	Prs.	Tmp.	Cctd	Cws	Cws-Cctd
27	75.0	5091.0	2.1035	32.7218	32.8172	0.07853

It is recommended that the residuals of the ssccv. RES file (last column above labelled Cws-Cctd) be examined both with station and pressure, as shown in Figures 8 and 9. Figure 9 includes observations from all pressure levels. By looking at the residuals versus station number, one can decide whether the conductivity data should be broken up into smaller groups or refit using the station-dependent conductivity slope option of program CONCALD. Notice that the average residual difference is indicated by a square on Figure 8 while the station standard deviation is indicated by a triangle. When the station average is significantly off the zero line, further examination of the individual stations is recommended to decide whether the problem lies with the CTD or water sample data. Often determining which salinity values are not consistent can be sorted out by plotting the water sample and CTD salinity versus potential temperature in the deep water (pressure > 2000 dbars) for neighboring stations as shown in Figure 10. The water sample and CTD salinity overplot versus potential temperature also provides a final data calibration check. Differences of the downprofile CTD salinity versus up-profile water salinity may indicate hysteresis in one of the parameters (pressure, temperature, or conductivity) that forms salinity. To insure that no vertical calibration problems exist in the CTD conductivity calibration, the residuals are also plotted versus pressure as shown in Figure 9. Small vertical deviations in the conductivity residuals may be due to vertical separation of the Niskin bottles above the CTD sensors (1.5 meters) in the presence of a vertical salinity gradient. For example, in the mid-latitude North Atlantic) the salinity gradient in the upper 1000 meters is roughly 0.002 psu per meter.

Oxygen

The WHOI conductivity-temperature-depth (CTD) instruments are all equipped with a polarographic dissolved oxygen sensor. This section describes the procedures for converting the CTD oxygen sensor measurements into oxygen profiles using the oxygen algorithm of Owens and Millard (1985) and in situ oxygen data from the discrete samples. The material in this section is adapted from the WHP Operations and Methods Manual (Millard, 1991).

The polarographic oxygen sensor first described by Kanwisher (1959) has been used in oceanography for thirty years. The most commonly used oxygen sensor is manufactured by Beckman (now Sensor Medics), and a thorough discussion of this sensor's behavior is given by Greene et al. (1970). The Beckman polarographic dissolved oxygen (DO) probe uses a gold cathode and silver anode electrode pair immersed in a KCl electrolyte through which current flows in proportion to the oxygen consumed.

The oxygen diffuses through a protective teflon membrane to reach the electrodes in quantities proportional to the surrounding oxygen. The teflon keeps the electrodes from fouling and reduces the probe's velocity sensitivity. The rate of diffusion of oxygen through the teflon membrane is temperature sensitive according to Greene, et al. (1970). The membrane temperature sensitivity requires a temperature measurement inside the polarographic oxygen sensor. While collecting cruise data, keeping the oxygen sensor membrane damp and clean (i.e., free of oil contamination) between stations is essential for good, stable oxygen measurements.

The following algorithm for converting the polarographic oxygen sensor oxygen current and probe temperature measurements to oxygen (Oxm) is described by Owens and Millard (1985):

$$Oxm = \left[A \cdot \left(Oc + B \cdot \frac{dOc}{dt}\right) + C\right] \cdot Oxsat(T, S)e^{D \cdot [T + E(To - T)] + F \cdot P}$$
 (19)

where Oc is the oxygen current measurement;

P and T are CTD pressure (dbar) and temperature (°C);

To is the oxygen sensor temperature (°C);

S is salinity computed on the 1978 practical salinity scale;

A is the oxygen current slope, B the oxygen sensor lag in seconds; and C is the oxygen current bias.

The three parameters (D, E, and F) appearing in the exponential are the teflon membrane temperature sensitivity adjustments and the adjustment for the hydrostatic pressure effects on the activity of oxygen. The pressure effect predicted from the ideal gas equation and data of Enns et al. (1965) is given as F = 0.000141. This analysis also suggests a cross-term involving pressure and temperature in the exponent but the effect is small (less than a 0.4 percent change in the resultant oxygen and nearly a constant with depth) and neglected. Oxsat(T, S) is the oxygen saturation value which uses the algorithm of Weiss (1970) in units of ml/l for the examples shown. The adoption of the Benson and Krause (1984) oxygen saturation formula is recommended by the Joint Panel of Oceanographic Tables and Standards (UNESCO, 1986) as it incorporates improved oxygen solubility measurements.

The Calibration Data:

Calibration data are required in order to determine the coefficients (A-F) of the algorithm shown in equation 19. Calibration in the laboratory has not been successful at yielding useful field calibration parameters because of the lack of stability of the DO sensor and perhaps also the lack of inclusion of pressure dependence in the laboratory calibration. Instead, in situ oxygen samples are collected during CTD profiles using a rosette multisampler or other water sample collection methods. The water sample oxygen data are currently analyzed by titration using the modified Winkler method (Carritt and Carpenter, 1966) with a conductivity end-point detection tech-

nique (Knapp et al., 1990). The analytical results from these samples are used for calibration.

The water sample oxygens are first merged with the appropriate CTD observations to be calibrated. It has been found that calibrations derived from the up-profile CTD data collected when stopped to fire the rosette do not apply well to the down-profile CTD data because the instrument is stopped and the DO probe is flow-sensitive at small lowering rates [< 0.4 m/s]. In general, down-profile CTD data are merged with corresponding up-profile water samples, either at common potential temperature levels or more commonly at corresponding pressure levels. After water sample data entry, the water sample oxygen data are quality controlled using property/property plots, such as potential temperature versus oxygen or by comparing with the oxygen saturation values near the surface. After correcting erroneous data entries, any other suspect oxygen data are flagged (see WHPO 90-1, Joyce, editor).

The units of CTD oxygen obtained using this oxygen fitting procedure are set by the units of the input water sample oxygens and oxygen saturation values. To conform to the WOCE recommended oxygen units, one need only provide water sample and oxygen saturation values in $\mu mol/kg$ as input data to program OXFITMR.

The calibration of oxygen sensor data is weakly dependent on the calibration of CTD pressure, temperature and conductivity (salinity) to the following extent. A maximum error of one percent in CTD oxygen results from a temperature error of 0.25°C (in either temperature sensor used in the oxygen algorithm), or a pressure error of 50 decibars, or a salinity error of 1 psu. It is recommended that the calibration of pressure, temperature and conductivity (salinity) be carried out prior to the oxygen calibration step.

Determining Coefficients of the Algorithm:

Use of equation 19 requires a non-linear least-squares regression technique in order to determine the best fit coefficients of the model for oxygen sensor behavior to the water sample observations. The program OXFITMR uses Numerical Recipes (Press et al., 1986) FORTRAN routines MRQMIN, MRQCOF, GAUSSJ, and COVSRT, to a perform a non-linear least squares regression using the Levenberg-Marquardt method. The Numerical Recipes FORTRAN routines MRQMIN and MRQCOF have both been slightly modified for use in program OXFITMR. The changes to these routines are given in (Millard, 1991). The purchase of a copy of the book, Numerical Recipes, entitles the owner to a machine-readable—py of these routines. A FORTRAN subroutine (FOXY) describes the oxygen model with the derivatives of the model with respect to the six coefficients.

The program reads the data for a group of stations which are selected as described below. The time rate of change of oxygen current $\frac{dOc}{dt}$ has been found to be adequately determined using a least squares estimate over 10 to 15 second intervals. Normally all of the oxygen data for a given oxygen probe and cruise are initially fit as a

single group. The data are edited to remove spurious points, i.e., values less than a threshold oxygen value (OXMIN) or greater than a factor larger than unity (default is 1.2) times the saturation value. The data removed by editing are recorded in an output file of rejected observations. The routine varies the six (or fewer) parameters of the model in such a way as to produce the minimum sum of squares in the difference between the calibration oxygens and the computed values.

Individual differences between the calibration oxygens and the computed values (residuals) are then compared with standard deviation σ of the residuals, and any residual exceeding an edit factor of 2.8σ is removed and stored in the reject file before refitting the data. The edit factor has a default value of 2.8 but can be changed so as to minimize rejecting valid data while still eliminating erroneous values. A factor of 2.8 will have a 0.5% chance of rejecting a valid oxygen value for a normally distributed set of residuals. The iterative fitting process is continued until none of the data fails the edit criterion and the best fit to the oxygen probe model coefficients is then determined. The oxygen residuals of the final fit are stored together with station number and other measured variables in an output file. By plotting the oxygen residuals versus station, the correct station groupings for further refinements of fitting are obtained. A sample plot of oxygen fit residuals versus station number is shown in Figure 11. Sample data from file HE06_74.RES used in this plot are found at the end of this section.

The average oxygen residual for each station is indicated with a square, while the standard deviation is given as a triangle. For a well-behaved DO probe, station groupings of between 10 and 30 stations are typical. The calibration coefficients (A - F) are stored, together with a histogram of the final fit residuals, in a histogram file. An example histogram for file HE06_74.HIS associated with the data of figure 11 is found near the end of this appendix. The standard deviation σ and the histogram of residuals are an indication of the goodness of fit. A normal distribution indicates that the fit describes all of the oxygen variation except the measurement uncertainty. When the distribution of residuals is not normal, a plot of the residuals versus pressure or alternatively temperature can be helpful in deciding the nature of the problem with the fitting procedure. Figure 12 illustrates a well-behaved set of residuals plotted versus pressure.

Some of the algorithm coefficients have a limited range of values which are reasonable. For example, the oxygen sensor lag parameter (B) should be restricted to positive values with a value in the range of seconds, not hundreds of seconds. The oxygen temperature difference parameter (E) should be bounded between 0 and 1.0 to represent a weighted membrane temperature. The following values for the various algorithm coefficients have been found to be typical.

Parameter		Typical Value
A		$0.0015 \ / \mu A$ for a deck unit reading in air of roughly $Oc \sim 1.1$
В	=	5.0 seconds
C	=	-0.01 (non-dimensional)
D	=	-0.035 /°C
${f E}$	=	0.75 (non-dimensional)
F	_=_	0.00015 /dbar

The file of oxygen data rejected by the fitting procedure, example HE06_74.REJ shown at the end of this appendix, can be helpful to the hydrographic group for further quality control of the water sample data. The oxygen residuals are differences defined as water sample oxygen minus the DO sensor value using the algorithm, so large differences indicate only that one or the other value is possibly erroneous. A large negative oxygen residual indicates that water sample oxygen is low or that the DO sensor value is high.

When attempting to fit very small station groups (less than 5 stations), it is sometimes helpful or necessary to pre-set some of the DO algorithm parameters. The parameters are arranged in the program to allow the most commonly pre-set parameters to be fixed while the others are adjusted. The pre-setting of a parameter may be supported by special constraints of the water sample oxygen data. For example, if the water sample oxygen is zero for portions of the profile, then any reading of the DO probe current must be compensated with an oxygen current bias of opposite sign, thus fixing the oxygen bias value if a zero oxygen value is to be achieved.

Details of the Water Sample Oxygen File to Fit:

The following water sample data format is used by the oxygen fitting program OX-FITMR. The file format is intended only to suggest the information required by the data fitting program. Notice that the oxygen current (Ox cur.) values in the table below and in the examples in the back are the nominal oxygen current values multiplied by 0.0014. Program OXFITMR prompts for this scaling value.

Pres.	Temp.	Ox Cur.	Ox Tmp.	Ox-WS	Ox-Sat	Doc/Dt	Descent Rate	Station .Bottle
dbars	°C	μA	°C	μmol/kg *	μ mol/kg *	$\mu A/s$	dbars/s	#
1.3	30.471	0.886	30.03	197.06	190.10	0.01080	0	55.11
59.1	29.006	1.142	30.34	195.95	192.71	-0.00001	0	55.10
159.0	23.901	0.795	29.96	143.99	203.30	-0.00690	0	55.09

^{*} Note: To obtain oxygen calibrations in units of $m\ell/\ell$, specify data columns Ox-WS (water sample oxygen) and Ox-Sat (oxygen saturation) in units of $m\ell/\ell$.

Examples of Files used for Oxygen Data Evaluation

Program OXFITMR was run on the ssccv. WSD file for stations 74 through 80 of Hesperides Cruise 6.

The following is a partial list of the input data used to produce the calibrations that follow: Note that the ssccv.WSD file pressure and temperature are the best calibrated CTD values while the CTD oxygen current is nominally scaled to engineering units (slope = .0014). The water sample oxygen is obtained by titration of the water samples. The oxygen saturation is computed from the CTD temperature and bottle salinity (set equal to 35 psu if out of range).

Input file:

TYPE HE06_74.0XY

press.	tempt.	oc	ot	ox(ws)	oxsat	DOC/DT	DP/DT	sta.
========	=======================================	======	======	=======	======	=======================================		======
25.1	28.523	2.844	30.85	4.65	4.41	-0.00125	0.2414	74.24
51.0	24.488	2.886	30.85	5.16	4.73	0.00075	0.7767	74.23
100.9	22.076	2.574	29.57	4.77	4.94	-0.01162	0.7703	74.22
123.0	21.078	2.327	28.73	4.56	5.03	-0.00693	0.7667	74.21
151.0	20.072	2.141	27.64	4.61	5.11	-0.00427	0.7767	74.20
175.1	19.610	1.997	26.64	4.42	5.17	-0.00246	0.7720	74.19
198.7	19.120	1.917	25.68	4.42	5.20	-0.00256	0.7713	74.18
249.3	18.506	1.828	23.90	4.48	5.26	-0.00178	0.7573	74.17
300.7	18.081	1.764	22.59	4.44	5.31	-0.00012	1.3631	74.16
403.0	16.950	1.574	21.12	4.20	5.45	-0.00310	1.3936	74.15
499.1	15.160	1.323	19.80	3.87	5.65	-0.00358	1.2248	74.14
601.1	13.262	1.222	18.05	4.10	5.86	-0.00221	1.2524	74.13
803.0	9.395	0.838	14.18	3.58	6.39	-0.00170	1.2332	74.12
999.0	6.704	0.731	10.51	3.90	6.81	0.00027	1.1792	74.11
1496.9	4.523	0.832	5.32	5.77	7.16	-0.00011	1.1941	74.10
1878.9	3.890	0.758	3.97	5.74	7.28	-0.00008	1.1653	74.09
2502.7	3.081	0.663	2.90	5.84	7.43	-0.00020	1.3126	74.08
3001.0	2.761	0.597	2.49	5.85	7.49	-0.00014	1.2656	74.07
3501.0	2.488	0.551	2.27	5.95	7.55	-0.00006	1.2864	74.06
4000.9	2.318	0.508	1.97	6.01	7.58	-0.00010	1.1847	74.05
4501.0	2.265	0.471	1.87	6.05	7.59	-0.00013	1.1347	74.04
4995.0	2.093	0.416	1.79	5.84	7.62	-0.00013	1.0604	74.03
5499.1	2.014	0.371	1.63	5.71	7.64	-0.00006	0.9542	74.02
5905.1	2.053	0.349	1.61	5.69	7.63	-0.00001	0.5945	74.01
9.0	28.482	2.459	26.24	4.57	4.42	0.00524	0.2514	75.24
50.9	23.320	2.657	26.94	5.23	4.80	-0.00001	0.7136	75.23
101.0	21.048	2.411	26.36	4.90	5.04	-0.00455	0.7154	75.22

Output files:

159

AVERAGE =

-0.000526

The following are examples of the histogram, residual, and reject files created by program OXFITMR.

The histogram file below is created by fitting for all six oxygen algorithm parameters for stations 74–80. Notice that at iteration 4 no further reject data were identified and that following the best fit oxygen algorithm parameters, a histogram is shown with a standard deviation of 0.066 ml/m.

```
TYPE HE06_74.HIS
Edit Fact= 2.80 Histo Bin= 0.2500E-01 OcSlope= 0.1400E-02
  1 Min/Max Sta: 74.- 80. 1 StdDev: 0.1264E+00 #0bs: 161 d0x: 0.354
         1: Bias
                 2:Slope
                            3:Pcor
                                     4:Tcor
                                               5: Wt
                                                         6: Lag
           2 Min/Max Sta: 74.-
                    80.
                         1 StdDev: 0.7487E-01 #0bs:
                                                 160 d0x: 0.210
         1: Bias
                 2:Slope
                            3:Pcor
                                     4:Tcor
                                               5: Wt
 OX Parms:
           3 Min/Max Sta: 74.- 80. 5 StdDev: 0.6737E-01 #0bs: 159 d0x: 0.189
         1: Bias
                 2:Slope
                            3:Pcor
                                     4:Tcor
                                               5: Wt
                                                         6: Lag
 OX Parms:
           0.026  0.1202E-02  0.1519E-03  -0.2865E-01  0.8885E+00  0.1029E+02
  4 Min/Max Sta: 74.- 80. 5 StdDev: 0.6576E-01 #0bs: 159
                                                     d0x: 0.184
         1: Bias
                 2:Slope
                            3:Pcor
                                     4:Tcor
                                               5: Wt
                                                         6: Lag
 OX Parms:
           0.027  0.1201E-02  0.1515E-03 -0.2865E-01  0.8869E+00
                                                         0.1027E+02
CLASS INT:
           0.025000
  -7
  -6
  -5
      10*******
  -4
       6****
  -3
  -2
  -1
   3
       4***
       4***
       2**
       2**
```

STD DEV. =

0.065967

The following is a partial list of those data included in the final fit procedure. The residual in column 7 is plotted versus station number (column 2) and pressure (column 3) to determine how well the CTD conductivity matches the water samples.

Type HE06_74.RES

Type nEub_/4	. RES					residual
	0 1 - 4	D	T	0	Owest	
doc/dt	Station	Prs.	Tmp	0x_ctd	Oxsat	Oxws-Oxctd
1250E-02	74.24	25.10	28.52	4.650	4.410	0.1225
0.7500E-03	74.23	51.00	24.49	5.160	4.730	0.1128
1162E-01	74.22	100.9	22.08	4.770	4.940	0.7028E-01
6930E-02	74.21	123.0	21.08	4.560	5.030	0.3273E-01
4270E-02	74.20	151.0	20.07	4.610	5.110	0.1765
2460E-02	74.19	175.1	19.61	4.420	5.170	0.6778E-01
2560E-02	74.18	198.7	19.12	4.420	5.200	0.9364E-01
1780E-02	74.17	249.3	18.51	4.480	5.260	0.5166E-01
1200E-03	74.16	300.7	18.08	4.440	5.310	1053
3100E-02	74.15	403.0	16.95	4.200	5.450	1293
3580E-02	74.14	499.1	15.16	3.870	5.650	9618E-01
2210E-02	74.13	601.1	13.26	4.100	5.860	4552E-02
1700E-02	74.12	803.0	9.395	3.580	6.390	0.1127E-01
0.2700E-03	74.11	999.0	6.704	3.900	6.810	0.3494E-02
1100E-03	74.10	1497.	4.523	5.770	7.160	0.4957E-01
8000E-04	74.09	1879.	3.890	5.740	7.280	1046
2000E-03	74.08	2503.	3.081	5.840	7.430	9001E-01
1400E-03	74.07	3001.	2.761	5.850	7.490	5483E-01
6000E-04	74.06	3501.	2.488	5.950	7.550	4634E-01
1000E-03	74.05	4001.	2.318	6.010	7.580	4833E-01
1300E-03	74.04	4 501.	2.265	6.050	7.590	5661E-01
1300E-03	74.03	4995.	2.093	5.840	7.620	5681E-01
6000E-04	74.02	5499.	2.014	5.710	7.640	6253E-01
1000E-04	74.01	5905.	2.053	5.690	7.630	1148
0.5240E-02	75.24	9.000	28.48	4.570	4.420	0.4611E-01
1000E-04	75.23	50.90	23.32	5.230	4.800	0.1152E-01
4550E-02	75.22	101.0	21.05	4.900	5.040	1300
5970E-02	75.21	176.9	19.38	4.590	5.200	0.5573E-01
2400E-03	75.20	252.9	18.42	4.580	5.280	6166E-01
2830E-02	75.19	353.1	17.46	4.410	5.390	1176
0.7100E-03	75.18	479.1	15.39	4.340	5.620	1227

The following is a list of those data excluded from the final fit procedure. This file is also reviewed by the hydrographic group since the water sample data is possibly erroneous.

Type HE06_74.rej

Prs	Tmp	0x_ws	Residual	Doc/dt	0xsat	Sta No.
150.9	22.35	-9.000	0.0000E+00	-4.014	4.910	79.21
200.9	20.24	-9.000	0.0000E+00	-1.836	5.130	79.20
3555.	2.442	-9.000	0.0000E+00	4286E-01	7.550	79.06
74.90	22.84	4.800	3593	2710E-02	4.910	76.22
10.90	28.42	4.660	9539	0.2597E-01	4.420	77.24
51.10	26.12	4.550	4077	2800E-03	4.610	79.23
606.9	13.54	3.920	1957	1390E-02	5.860	77.16

Appendix 5: Examples of Data Files Used in PC Processing

All of the PC post acquisition data files are ASCII with the exceptions of the unscaled binary CTD data file illustrated in the hexidecimal dump of file HE06D050.EDT below. The first six file print outs listed in Appendix 5 are associated with CTD data processing. Sample printouts seven through nine are associated with water sample data file formats. Examples of conductivity (salinity) and oxygen calibration file formats can be found in Appendix 4.

**** CTD Data Processing Files *****

1 ****** HE06D050.EDT **** binary unscaled CTD data

This is a binary data file containing the unscaled CTD data with suspect data values marked in quality bytes. Note that the hexidecimal dump is of a data file for a standard Mark IIIb CTD with an 11 byte data sequence telemetered from the CTD with two bytes added by CTDACQ for data quality indicator bytes. The frame syncronization byte alternates 0F and F0 hex and the first 5 occurrences are underlined below.

Dump of file CTDA:<CTDEV.PRSAVG>XI06D001.EDT;2 on 22-JUN-1990 11:49:38.66 File ID (9117,3,0) End of file block 173 / Allocated 175

Record number 1 (00000001), 512 (0200) bytes

33C91E00 68F00020 CC06B401 0033C91E 00640F00 00CC06B4 010033C9 1E0065F0 20CC06B4 010033C9 1F0068F0 0020CC06 B4010033 C91F0065 0F0020CC 06B40100 C9200063 0F0020CC 06B40100 33C92000 61F00020 CC06B401 0033C920 00680F00 CC06B401 0033C921 00630F00 20CC06B4 010033C9 210063F0 0020CC06 B4010034 220062F0 0020CC06 B4010033 C9220062 0F0020CC 06B40100 34C92200 62F00020 06B40100 33C92300 63F00020 CC06B401 0033C923 00620F00 20CC06B4 010033C9 00630F00 20CC06B4 010033C9 240064F0 0020CC06 B4010033 C9230065 0F0020CC B4010034 C9250063 OF0020CC 06B40100 34C92400 63F00020 CC06B401 0034C924 63F00020 CC06B401 0034C925 00650F00 20CC06B4 010034C9 260063F0 0020CC06 010034C9 260064F0 0020CC06 B4010034 C9260064 0F0020CC 06B40100 34C92600 0F0020CB 06B40100 34C92700 68F00020 CC06B401 0034C927 00640F00 20CC06B4 0034C928 00640F00 20CB06B4 010034C9 280063F0 0020CB06 B4010034 C9270065 0020CB06 B4010034 C9280063 0F0020CB 06B40100 34C92800 63F00020 CB06B401 34C92A00 65F00020 CB06B401 0034C92A 00650F00 20CB06B4 010034C9 290063F0 20CB06B4 010034C9 2A0063F0 0020CB06 B4010034 C92A0066 0F0020CB 06B40100 C92C0064 0F0020CB 06B40100 34C92B00 63F00020 CB06B401 0034C92B 00650F00

```
2 ******* HE06D050.C00 ***********
                    COMMUNICATIONS PARAMETERS
                                                         ; 9600,N,8,2
                    RECORD LAYOUT; SS-1,02-2,03-2,04-2,UU-1,06-2,07-1,14-2,TT-0
                    DIGITIZER OPTION; 14 [14,10]
                    IDLE BITS
                                                          ; 0
                    UTILITY BYTE LAYOUT
                                                          ; 12500000
                                                          ; 31.25
                    SCAN RATE
  *B
                    CALIBRATION LABORATORY DATA
                    CALIBRATION S/N
                    CALIBRATION FACILITY
                                                         ; Woods Hole
                    TECHNICIAN
                                                          ; Gary Bond, CTD
                    DATE
                                                          ; June 30 1992
  *C
                    INSTRUMENT CONFIGURATION DATA
                                                       Spanish 2nd CTD
                    UNIT SERIAL NUMBER
                                                         ; 1101-01
                    SENSOR HEAD S/N
                    DATE LAST PHYSICAL CALIBRATION
                    DATE LAST ELECTRICAL SET-UP
  *2
                    PRESSURE
                    STANDARD PRESSURE S/N
                                                          ; 157766
                    DATE LAST STANDARD CALIBRATION
                    PRESSURE SENSOR S/N
                                                         ; 157766
                    P,T,C, INTERFACE S/N
                    DATE LAST PRESSURE CALIBRATION ; June 1992
                    A ; 0.0
                    B; 0.000000E+00
                    C; 0.593893E-09
                    D; 0.108604E+00
                    E; -.107536E+01
                  LAG ; +0.000000E+00
                  LAG'; +0.000000E+00
```

ACQLAG; 0.0

*3

TEMPERATURE

```
STANDARD TEMPERATURE S/N (ATB-1250)
                                                      ;1021
                  SPRT SENSOR S/N
                  DATE LAST STANDARD CALIBRATION
                  PLATINUM TEMPERATURE SENSOR S/N
                  P.T.C INTERFACE S/N
                  DATE LAST TEMPERATURE CALIBRATION ; June 30 1992
                  A : 0.0
                  B; 0.0
                  C; 0.195371E-11
                  D; 0.499476E-03
                  E; -0.414012
                LAG ; 0.22500000
                LAG': +0.000000E+00
              ACQLAG; 0.0
*4
                  CONDUCTIVITY
                  CONDUCTIVITY STANDARD S/N
                                                        ; CSA-1250
                  CONDUCTIVITY INTERFACE S/N
                  CONDUCTIVITY SENSOR S/N
                  DATE LAST STANDARD CALIBRATION
                  CONDUCTIVITY SENSOR S/N
                  P,T,C,INTERFACE S/N
                  DATE LAST CONDUCTIVITY CALIBRATION ; June 1992
                  A ; 0.0
                  B; 0.0
                  C; 0.0
                  D; 0.100024E-02
                  E ; -0.11600E-01
                LAG ; +0.000000E+00
                LAG'; +0.0000000E+00
              ACQLAG; 0.0
        ALPHA -6.5E-6; -6.4999999E-06
         BETA 1.5E-8 ; 1.499999E-08
                  TO; 2.800000
                  PO: 3000.000
```

* N

Notations:

Spanish modified Mark III CTD with Oxygen current and temperature, plus titanium pressure sensor with RTD added by WHOI CTD group G. Bond in June 1992.

3 ******** HE06D050.HDR **********

Besides representing a separate data file with an extension of _____.HDR, the header file information is at the beginning of the following files (_____.BTL, ____.PRS, ____.P10)

Vessel: Hesperides | Cruise \#:6

Sta.\#:50 | Operator: THE X-TEAM!!

CAL Extn: COO | Date: 02-AUG-1992 St.Time: 02:35:01 | En.Time: 03:19:40 St.Lat.:24 :30:12.60 | En.Lat.:24:30:3.34 St.Long:-44 :40:4.40 | En.Long:-44:40:11.19 Depth:3000 Meters | Obs.: 84124 : | ScanRate: 31.25 Hz

PRES >,<: 2.0 2998.8|TEMP >,<: 2.732326.6803 COND >,<:-0.011658.6145|OXCU >,<: 0.599 2.880 OXTM >,<: 2.176 25.600|PRTM >,<: 6.979725.9891

4 *** HE06D050.PRR **** 2 dbar pressure averaged data - unscaled except prs

P	T_R	C_R	OC_R	OT_R	TP_R	#obs
2.94	53926.30	58251.03	1895.96	196.50	598.00	128.00
5.00	54207.32	58581.05	1845.37	196.39	597.99	83.00
7.01	54215.44	58591.75	1840.80	196.40	598.00	100.00
8.87	54214.79	58593.42	1818.61	196.46	598.00	119.00
11.19	54219.11	58594.94	1814.88	196.99	597.09	1170.00
12.76	54220.88	58597.68	1828.18	197.91	597.00	160.00
•						
•						
2997.15	6300.26	32630.60	3 9 9.46	17.46	2815.82	57.00
2998.08	6300.64	32631.00	400.01	18.00	2818.79	498.00

5 ***** HE06D050.PRS ***** 2 dbar pressure centered data - scale with Salt and O2

" Header data - see HEO6D050.HDR"

PRES*	:	TEMP*		SALT*	OX	GY*	N	OBS	
3.0,	26	.5266,	37	7.5929,	4.8	33,	12	8	
5.0,	26	.6670,	37	7.7180,	4.8	19,	8	3	
7.0,	26	.6711,	37	7.7218,	4.8	20,	10	0	
9.0,	26	.6708,	37	7.7227,	4.8	20,	11	9	
11.0,	26	.6728,	37	7.7213,	4.8	15,	117	0	
•									
•									
•									
•									
2993.	Ο,	2.732	В,	34.9372	, 5	.651	,	163	
2005	^	0 730		24 0271	_	650		40	

2995.0, 2.7328, 34.9372, 5.651, 163 2995.0, 2.7328, 34.9371, 5.659, 48 2997.0, 2.7329, 34.9374, 5.649, 57

5b ***** HE06D050.P10***** 10dbar pressure centered data - scale with S/O2

' Header data - see HEO6D050.HDR"

PRES* TEMP* SALT* OXGY* NOBS
15.0, 26.6740, 37.7221, 4.5438, 1558
25.0, 26.6487, 37.7141, 4.5430, 292
35.0, 25.2757, 37.5283, 4.7784, 322
45.0, 24.5892, 37.5057, 4.9382, 301

2965.0, 2.7405, 34.9376, 5.5404, 261 2975.0, 2.7365, 34.9373, 5.5506, 247 2985.0, 2.7332, 34.9370, 5.5400, 425 2995.0, 2.7328, 34.9369, 5.5250, 835 6]****** HE06D050.LTG ********

2999

2.733 34.937

5.52

2.488

27.881

Station Listing

- 6 - 50 2- 8- 92 TIME: 2:35 LAT: DATE (D/M/Y): 24:30.21 LONG: -44:40.07 GRAVITY= 9.7889 M/S^2 CORIOLIS= 0.59331E-04 1/S SOUND SPEED = 1504.3 M/S Depth = 3000 Meters PRES TMP SALT OXYG PTMP SIG-TH SIG-2 SIG-4 DYN-HT PE GRD-PT GRD-S DENSITY B-V DEPTH DBAR С C/DB **PSU** ml/l C KG/M3 KG/M3 KG/M3 DYNAMIC J/M2 1/08 RATIO METERS **METERS** 10-5 10-3 10-3 5.00 0 26.045 37.180 4.61 26.045 24,667 32.925 40,832 0.000 0.0 -0.22 0.000 0.000 0.0 40.832 1 26.045 37.180 4.61 26.045 24.667 32.925 0.003 0.0 -0.45 0.000 0.00 0.000 10 26.672 37.722 4.52 26.670 33.115 41.002 0.19 24.878 0.031 0.0 0.050 3.59 -0.276 10.0 50 24.498 37.509 0.4 -34.74 4.95 24.487 25.397 33.691 41.631 0.147 -0.651 21,29 5.755 49.8 100 23.314 37.449 5.00 23.293 25.708 34.034 42.005 0.270 1.3 -33.94 -2.375 5.53 5.079 99.6 26.012 150 21.900 37.309 4.80 21.870 34.379 42.388 0.378 2.7 -29.04 -5.336 2.02 3.616 149.4 200 19.386 36.817 4.38 19.349 26.321 34.769 42.853 0.474 4.4 -38.75 -7.647 1,74 3.737 199.1 250 17.916 36.538 4.33 17.872 26.483 34.981 43.112 0.559 6.3 -16.86 -2.856 1.92 2.549 248.8 300 16.991 36.364 4.32 16.941 26.577 35.107 43.269 0.639 -20.06 8.6 -3.735 1.70 2.538 298.5 400 15.064 36.042 4.34 15.002 26.776 35.378 43.606 0.787 13.8 -14.27 -2.285 1.83 2.194 397.9 500 13.523 35.818 4.25 13.451 43.881 20.0 -19.79 497.2 26.935 35.597 0.921 -2.664 2.06 2.648 600 12.119 35.638 4.03 12.038 27.078 35.797 44.135 1.041 26.7 -11.89 -1.445 2.15 2.023 596.4 700 10.461 35.439 1,149 3.58 10.375 2.06 2.453 27.230 36.019 44.422 33.8 -19.26 -2.272 695.5 800 8.882 35.255 3.41 8.793 27.352 36.211 44.680 1,243 41.0 -14.51 -1.676 1.94 1.998 794.6 900 7.730 35.127 3.36 36.341 44.860 1.327 1.781 7.637 27.428 48.3 -11.33 -1.117 893.7 2.14 1000 6.636 35.030 3.54 6.539 27.506 36.471 45.039 1.404 55.8 -7.35 -0.468 3.12 1.584 992.7 1100 6.136 35.015 3.82 6.034 27.561 36.550 45.141 1.474 63.3 -3.83 -0.008 98.06 1.357 1091.6 1200 5.748 35.026 4.14 5.639 27.619 36.628 45.237 1.540 71.0 -3.51 0.279 -2.38 1.538 1190.5 1300 5.360 35.056 4.57 5.245 27.691 36.718 45.345 1.601 78.7 -3.36 0.282 -2.23 1289.3 1.523 1,656 1400 5.154 35.070 5.030 27.727 36.765 45.401 86.4 1388.1 4.80 -2.86 -0.004 100.00 1.160 1500 4.904 35.071 4.97 4.773 27.758 36.809 45.457 1.709 94.2 -2.89 -0.003 100.00 1.163 1486.9 1750 114.3 4.286 35.053 5.28 4.139 27.813 36.896 45.575 1.830 -1.91 1733.5 -0.097 3.56 0.813 3.833 35.023 2000 5.43 3.668 27.839 36.946 45.648 1.945 136.2 -1.67 -0.110 2.76 0.722 1979.8 2250 3.277 3.461 34.996 5.51 27.856 36.984 45.706 2.055 160.1 -1.67 -0.121 2.54 0.711 2225.8 2500 186.1 3.102 34.968 5.53 2.900 27.869 37.018 45.758 2.163 -1.47 -0.099 2.76 0.690 2471.6 2750 2.881 34.951 5.54 2.658 27.877 37.039 45.792 2.267 214.1 -0.81 -0.064 2.25 0.498 2717.1

45.814

2,372

244.7

37.052

-0.74

-0.059

2.24

0.000

2961.3

**** Rosette Bottle Files *****

7] ****** HE06U005.BTL ******* Rosette bottle data from CTDACQ

	41	Header da	ta - see	нс	OR"						
BT#	SCAN#	PRES	TEMP	COND	SALT*	LCOND	LSALT	oxcu	ОХТМ	OXYG*	FLUR
1,	2617,	1915.24,	3.95501,	33.36241,	35.02148,	,		0.6990,	3.3280,	5.9727,	
1,	2617,	17643.3,	8746.9,	33366.0,	35.02148,	•	•	466.0,	26.0,	5.9727,	
2,	2958,	1914.02,	3.95451,	33.36241,	35.02260,	,		0.9705,	3.3280,	8.2911,	
2.	2958,	17632.0,	8745.9,	33366.0,	35.02260,	•	•	647.0,	26.0,	8.2911,	
3,	4201,	1914.37,	3.95256,	33.36041,	35.02214			0.7125,	3.3280,	6.0877,	
.3,	4201,	17635.3,	8742.0,		35.02214,	•	,	475.0,	26.0,	6.0877,	
4	14941,	1722.11,	/ 2857 7	33.59646,	35 0/031			0.7023,	3.2233,	5.7806,	
4,	14941	15865.3,	9409.0,		35.04031,	•	•	468.2,	25.2,	5.7806,	
	45/74	4774 70	/ 20/02					·		•	
5, 5,	15431, 15431,	1721.29, 15857.7,	4.28482, 9407.2,	33.59510, 33598.6.	35.04007, 35.04007,		•	0.7875, 525.0,	3.3280, 26.0,	6.4632, 6.4632,	
•		•	· ·		-	•	•		20.0,	•	
6, 6,		1513.23, 13942.3,	4.89269, 10624.1,	34.09031,	35.07811, 35.07811,	•	•	0.6945, 463.0,	3.5840, 28.0,	5.3755, 5.3755	
0,	24327,		10024.1,			•	•	403.0,	20.0,	5.3755,	
7,		1414.34,	5.31696,			•	•	0.6900,	3.8400,	5.1517,	
7,	29838,	13031.9,	11473.5,	34407.2,	35.11447,	•	•	460.0,	30.0,	5.1517,	
8,		1311.89,	5.73960,			•	,	0.6825,	4.2240,	4.8971,	
8,	34476,	12088.6,	12319.5,	34828.6,	35.13400,	.*	•	455.0,	33.0,	4.8971,	
9,	39421,	1206.83,	6.27237,			,	,	0.6540,	4.6080,	4.4923,	
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10,	46980,	9293.9,	14800.2,		35.13237,	•		402.0,	41.0,	3.8627,	
11,	54410,	805.66	7.72588,	36.40732,	35.09800.	Ā	_	0.4980,	5.8880,	2.9703,	
	54410,	7427.9,	16295.8,		35.09800,	•		332.0,	46.0,	2.9703,	
12.	61094,	594.71,	9.92952,	38.63613,	35 35483			0.5820,	6.7840,	3.0580,	
	61094,	5485.7,	20707.1,		35.35483,	•	,	388.0,	53.0,	3.0580,	
13	66671,	510.04,	11.07147,	39.84387,	35 50/77			0.7725,	8.3200,	3.7088,	
13,	•	4706.1,	22993.0,		35.50477,	•	•	515.0,	65.0,	3.7088,	
47	72574	/00.70	10 771/0		_	·	•		0.05/0		
14,	72531, 72531,	409.30, 3778.5,	25595.1,	41.23130, 41233.0,	35.66853,	•	,	0.9266, 617.7,	9.8560, 77.0,	4.0375, 4.0375,	
		_				•	•	•		•	
15, 15.	78996, 78996,	306.29, 2830.1,	13.94195, 28738.8,	42.98208,	35.90027, 35.90027,	•	•	1.0920, 728.0,	11.2640, 88.0,	4.2986, 4.2986,	
			•			•	•	, 20.0,	٠٠.٠,	4.2,00,	
	82889,			44.40106,		•	•	1.3455,	12.4160,	4.9127,	
10,	82889,	2351.3,	31134.0,	44402.0,	36.12216,	•	•	897.0,	97.0,	4.9127,	
	87514,	202.59,	16.16734,	45.62826,		•	,	1.5000,	13.6960,	5.0909,	
17,	87514,	1875.3,	33193.2,	45628.9,	36.30600,	•	•	1000.0,	107.0,	5.0909,	
	91383,	152.60,	17.20512,	46.88629,		•	,	1.6725,	14.7200,	5.3147,	
18,	91383,	1415.0,	35270.4,	46886.6,	36.49367,	•	•	1115.0,	115.0,	5.3147,	
	93987,	126.10,	17.58601,	47.33303,	36.54912,	,	,	1.8135,	15.4880,	5.5602,	
19,	93987,	1171.0,	36032.7,	47333.3,	36.54912,	•		1209.0,	121.0,	5.5602,	
20,	96474,	102.25.	18.56072,	48.55433,	36.73279,	,		2.0850,	16.1280,	6.0854,	
20,		951.4,	37983.6,	•	36.73279,	•	;	1390.0,	126.0,	6.0854,	
21.	96743,	103.39	18.52052,	48.53796,	36.75435			3.6540,	16.2560,	10.6403,	
	96743,	961.9,	37903.2,		36.75435,	•	•	2436.0,	127.0,		

**** Rosette Bottle files *****

```
8] ***** HE06S005.BT2 ****** unscaled CTD with water sample S/02 merged

8b] **** HE06U005.BT2 *** same file above with -9.00 for WS S/02 last line below
```

5	1 1 -9.0000	4.948	17642.9	8747.0	33366.0 35.0215	466.0	26.0	5.973	2649.1 0.589	0.429E-01
5	2 2 -9.0000	-9.000	17632.5	8745.9	33366.0 35.0226	636.7	26.0	8.291	2681.0 0.861	1.97
5	3 3 35,0210	-9.000	17636.5	8742.0	33364.0 35.0221	475.0	26.0	6,088	2693.9 0.861	-0.243
5	4 4 35.0380	4.764	15865.4	9409.0	33600.0 35.0403	468.4	25.4	5.781	2847.3 0.368	0.786E-01
5	5 5 -9.0000	-9.000	15858.0	9407.3	33598.3 35.0401	522.7	25.7	6.463	2867.0 0.811	5.06
5	6 6 -9,0000	4.442	13942.2	10624.1	34093.6 35.0781	463.3	28.0	5.376	2937.0 0.218	0.357E-02
5	7 7 -9.0000	4.297	13031.9	11473.7	34469.2 35.1145	459.7	30.0	5.152	2967.7 0.125	-0.357E-02
5	8 8 -9.0000	3.992	12089.2	12319.4	34828.5 35.1340	454.8	33.0	4.897	2983.5 0.679E-01	
Š	9 9 35.1400	3.716	11122.1	13385.7	35287.1 35.1510	436.0	36.0	4.492	2990.0 0.179E-01	
5	10 10 -9.0000	3.240	9294.6	14800.3	35836.5 35.1324	402.0	41.0	3.863	2981.3 -0.607E-01	0.121
5	11 11 35.0850	2.570	7426.0	16293.3	36410.3 35.0980	332.0	46.0	2.970	2956.0 -0.136	-0.143
5	12 12 35.3400	2.630	5485.5	20705.1	38637.4 35.3548	388.5	53.0	3.058	2919.2 -0.211	0.907
5	13 13 35,4890	3.092	4707.6	22993.0	39845.9 35.5048	515.0	65.0	3.709	2866.0 -0.336	-0.307
Š	14 14 35.6520	-9.000	3777.0	25595.2	41233.0 35.6685	618.5	77.0	4.037	2785.8 -0.450	0.475
Ś	15 15 35.8820	3.583	2830.0	28739.1	42783.6 35.9003	728.0	88.0	4.299	2679.0 -0.496	-0.535E-01
Ś	16 16 36.0970	-9.000	2351.5	31134.2	44402.2 36.1222	897.5	97.0	4.913	2604.0 -0.579	1.26
5	17 17 36.2840	4.202	1875.5	33194.1	45629.0 36.3060	1000.4	106.9	5.091		
5									2507.5 -0.621	0.954
	18 18 36.4710	4.416	1414.8	35270.0	46886.0 36.4937	1115.0	115.0	5.315	2419.8 -0.668	1.09
5	19 19 36.5280	4.596	1171.6	36034.3	47333.5 36.5491	1208.0	121.0	5.540	2355.3 -0.743	1.13
5	20 20 -9.0000	5.092	952.9	37982.8	48553.7 36.7328	1391.9	126.0	6.085	2290.8 -0.811	0.871
5	21 21 36.7040	-9.000	961.4	37887.5	48518.5 36.7543	2436.0	127.0	10.640	2303.6 -0.550	13.2
5	22 22 36.5540	5.285	469.0	42630.7	50786.4 36.5708	1617.6	134.6	6.391	2184.1 -0.786	1.94
5	23 23 36.6220	5.116	260.8	44018.8	51607.8 36.6463	1608.1	143.0	6.047	2121.5 -0.986	-6.37
5	24 24 35.6220	5.163	82.4	44019.8	51596.6 36.6443	1679.2	158.0	5.995	1950.5 -0.871	0.643

**** Rosette Bottle Files (Continuation) *****

9]** HEO6U050.SOX *** scaled CID - water sample S/O2 merged by Hydro group 9b]** HEO6U050.TMP ** same above but -9.00 for WS S/O2 see last line below 9c]** HEO6U050.CTP *** scaled CID with water sample S/O2 plus down CID 02

All of these files are WOCE water sample format.

QUALT1		11111111	1111111111	1111111	1111111111	1111111111	1111111	1111111	1111111	1111111	1111111	1111111	1111111	1111111	1111111	1111111	1111111	1111111	1111111111	1111111	1111111	1111111	1111111	1111111	1111111
CFC-12	****	-9.000 1111111111	-9.000 111	-9.000 11111111111	-9.000 111	-9.000 111	-9.000 11111111111	-9.000 11111111111	-9.000 111111111	-9.000 1111111111	-9.000 11111111111	-9.000 1111111111	-9.000 11111111111	-9.000 11111111111	-9.000 1111111111	-9.000 1111111111	-9.000 1111111111	-9.000 1111111111	-9.000 1111	-9.000 1111111111	-9.000 1111111111	-9.000 1111111111	-9.000 1111111111	-9.000 1111111111	-9.000 11111111111
	*****	-9.000	-9.000	-9.000	-9.000	-9.000	-9.000	-9.000	-9.000	-9.000	- 0000.6-	000.6-	- 0000.6-	- 0000.6-	- 0000.6-	. 000.6-	- 000.6-	- 000.6-	. 000.6-	. 000.6-	. 000.6-	. 000.6-	- 0000.6-	. 000.6-	. 000.6-
PHSPHT	######################################	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00
NITRIT	III. GIROL/KU GIROL/KU GIROL/KU GIROL/KU GIROL/KU	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00
NITRAT	******	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	.9.00	-9.00	-9.00
SILCAT	******	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00	-9.00
OXYGEN	******	5.226	5.648	5.661	5.653	5.651	5.659	5.658	5.543	5.035	3.668	3.379	3.751	4.199	4.347	4.391	4.426	4.343	4.641	4.873	5.095	5.043	5.033	4.673	4.663
SALNTY	******	2.4890 34.9366	2.8393 34.9657	2.8459 34.9657	2.8364 34.9661	2.8385 34.9655	2.8447 34.9649	2.8502 34.9655	3.6169 35.0219	4.7869 35.1873	6.4363 35.0298	35.2120	35.5925	35.7629	36.0004	36.3170	36.4717	36.7087	37.2067	37.3544	37.4423	37.4939	37.5085	37.7205	37.7221
THETA	00-61-41	2.4890	2.8393	2.8459	2.8364	2.8385	2.8447	2.8502	3.6169	4.7869	6.4363	8.3793	11.6037 35.5925	13.0404 35.7629	14.6761 36.0004	16.5739 36.3170	17.3817 36.4717	18.5595 36.7087	21.0668	22.0970 37.3544	23.0526 37.4423	23.8820 37.4939	24.3893 37.5085	4.815 26.6438 37.7205	4.739 26.6521 37.722
CTBOXY	******	5.650	5.674	5.672	5.675	5.674	5.674	5.672	5.575	5.129	3.643	3.478	4.119	4.331	4.402	4.391	4.430	4.517	5.004	5.167	5.179	5.166	5.155	4.815	4.739
081692 CTDSAL	******	34.9369	34.9668	34.9655		34.9652	34.9647	34.9664	35.0207	35.0733		35.2082	35.5991	35.7668	36.0088	36.3042	36.4598	36.5025	37.2357	37.3660	37.4626	37.5197	37.5213	37.7226	37.7235
CRUISE DATES 071492-081692 DRAW CIDPRS CIDIMP CIDS	doars ifistoo	2.7337	3.0434	3.0500	3.0404	3.0425	3.0489	3.0544	3.7835	4.9194	9	£297	E.	<u>o</u> .	404.4 14.7375	305.2 16.6241	256.1 17.4252	204.6 18.5958	152.1 21.0963	127.2 22.1226	101.9 23.0737	76.5 23.8982	52.1 24.4005	27.5 26.6501	12.0 26.6549
CTDPRS	STBOD	2996.4	2531.8	2531.1	2531.9	2531.1	2533.2	2531.9	2021.3	1516.6	1012.5	809.9	909	507	404.4	305.2	256.1	204.6	152.1	127.2	101.9	76.5	52.1	27.5	12.0
CRUISE		27598.5	23321.8	23314.9	23321.3	23313.1	23333.1	23319.7	18622.1	13976.1	9335.5	7469.9	5596.4	4685.5	3733.8	2820.0	2366.8	1893.1	1406.7	1176.6	945.8	709.0	486.3	258.5	115.5
WHP-ID WOCE SAMPNO BTLNBR	*****	-	2	M	4	2	9	7	€0	٥	10		12	5	14	15	5	17	2	19	20	21	22	23	54
		7	ĸ	4	50	9	7	80	6	10	7	12	13	14	15	16	17	18	19	20	21	22	23	57	23
EXPOCODE 31HEO6 STNNBR CASTNO		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
EXPOCODI STNNBR		S	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	· 05	20

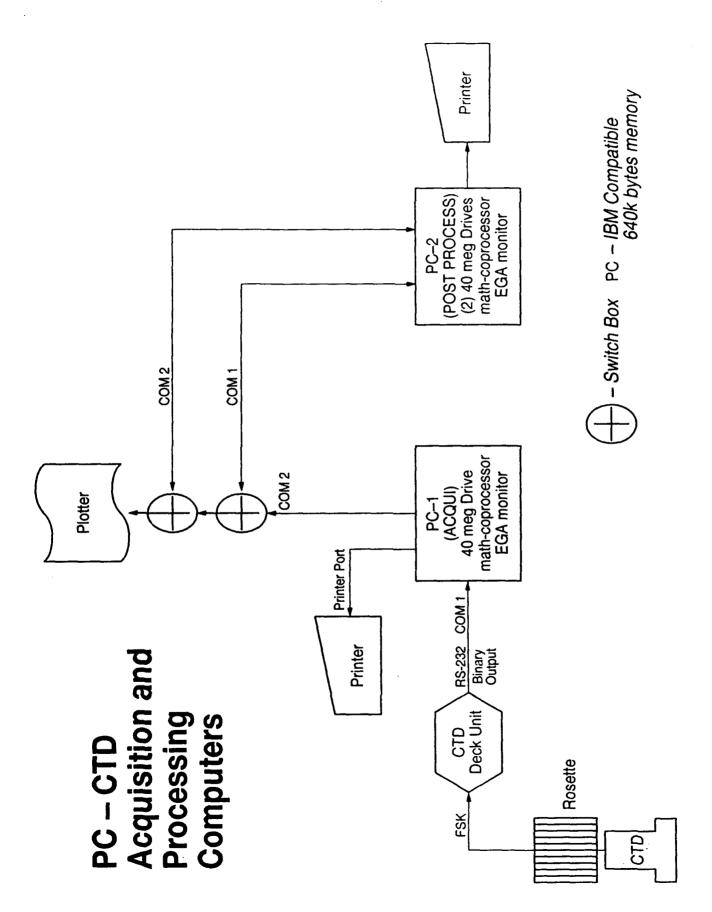


Figure 1: Diagram of interconnections between two interchangeable PC's as normally set up to allow post processing on spare computer while data logging on primary computer. 24-pin or laser printer also serves as graphics device.

Laboratory Calibration Data (CREATE INSTRUMENT CALIBRATION FILE)

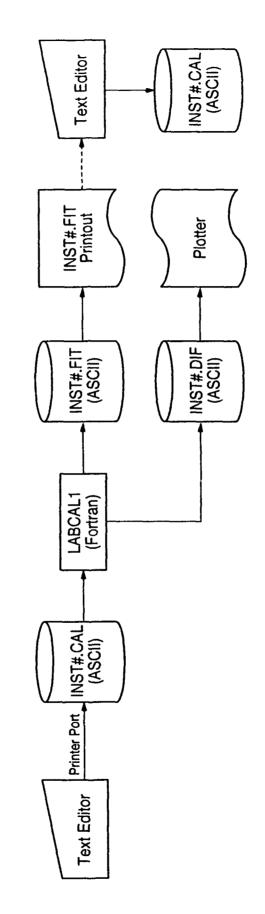


Figure 2: Sequence of data processing steps to determine laboratory calibration coefficients entered into instrument calibration file.

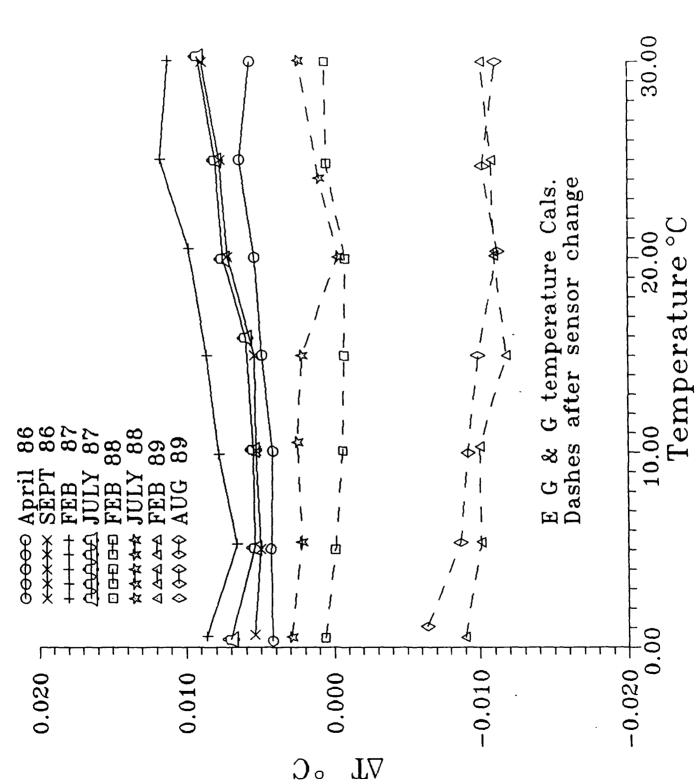


Figure 3: EG&G Mark IIIb temperature sensor calibration variations between April 1986 and September 1989.

Water Sample Merge

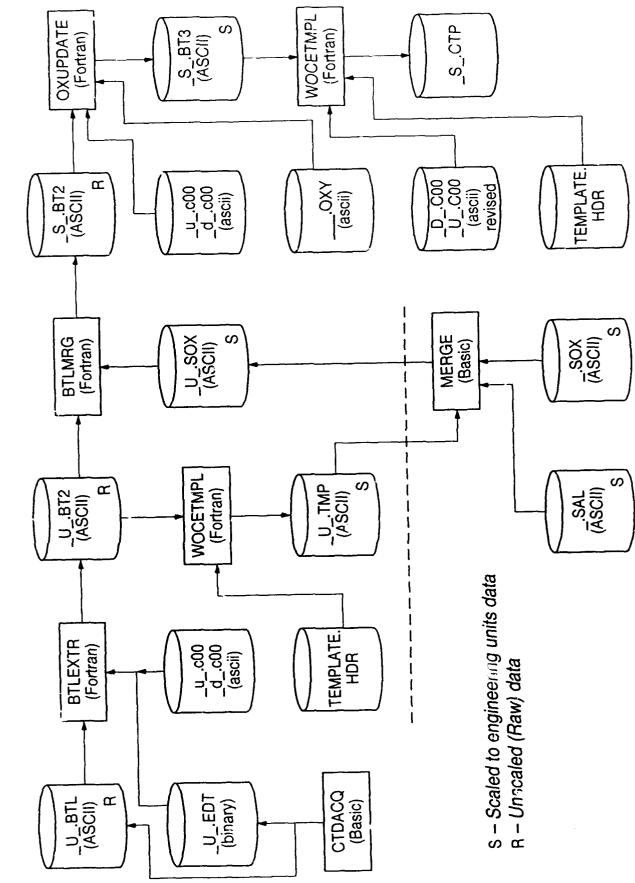


Figure 4: Water sample processing sequence used to prepar CTD observations at rosette observation levels for water sample analysis groups/ data archives and CTD calibration on the PC.

Calibration of CTD Conductivity (Salinity) to Water Samples

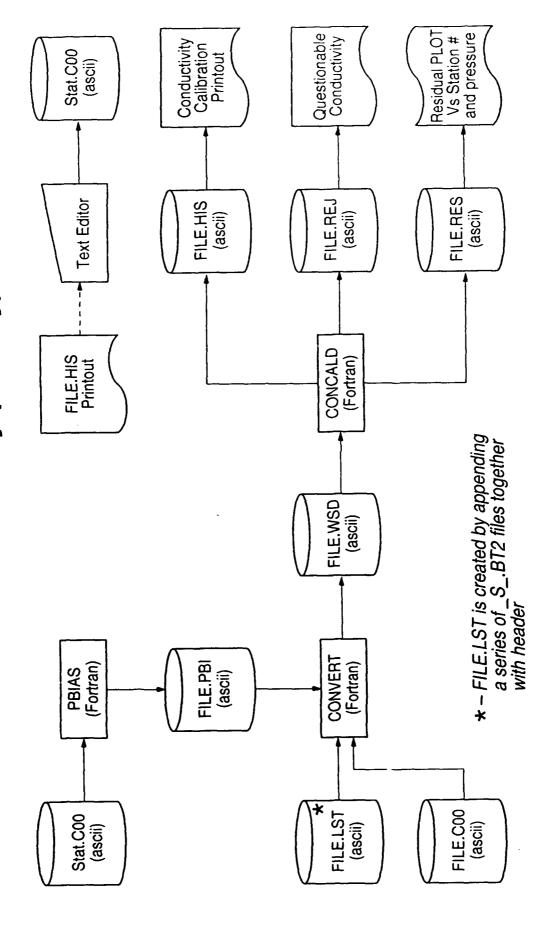


Figure 5: Fitting procedure used to determine the CTD conductivity calibration coefficients from in situ water sample salinities inverted to conductivity.

Calibration of CTD Oxygen with Water Samples

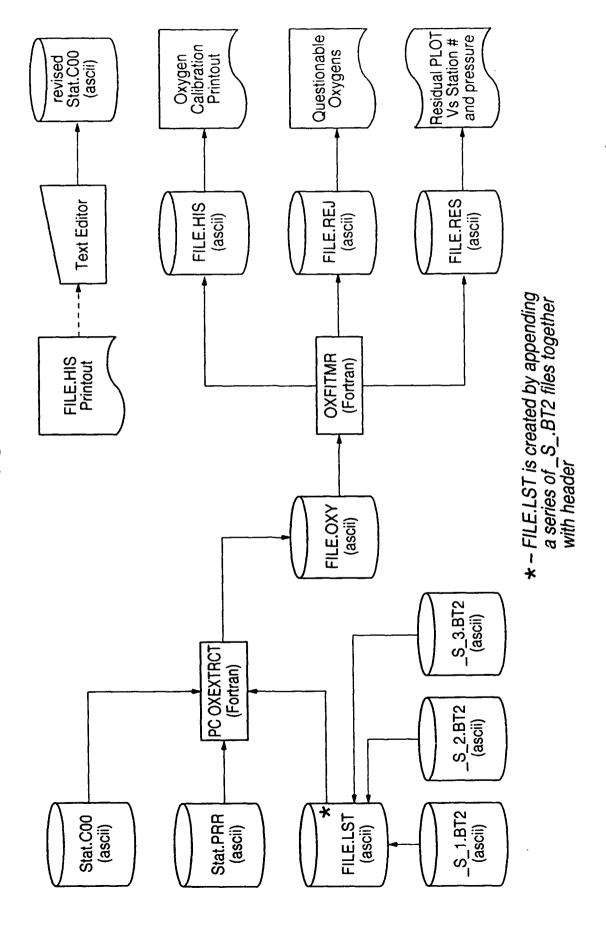


Figure 6: Fitting procedure used to determine the CTD oxygen algorithm calibration parameters from in situ water sample oxygens.

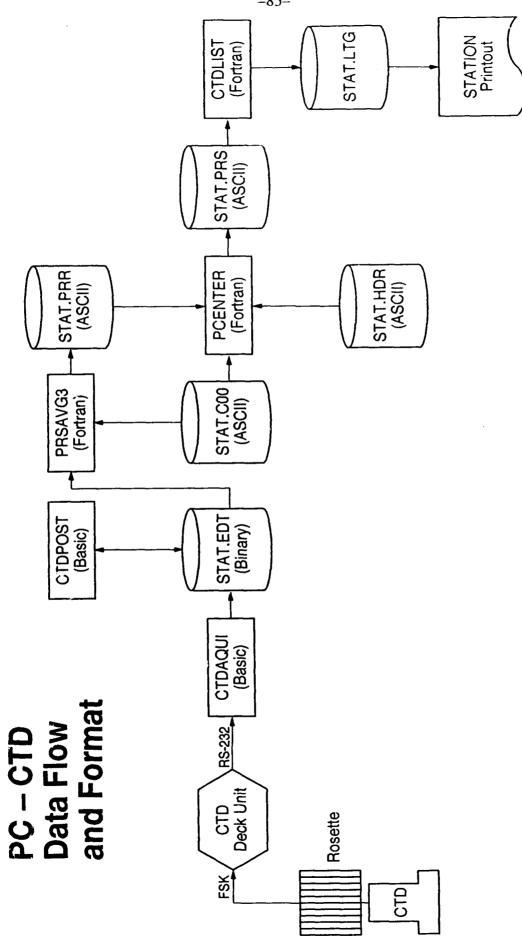


Figure 7: A schematic of the CTD data flow from acquisition to a uniform pressure data file for the PC.

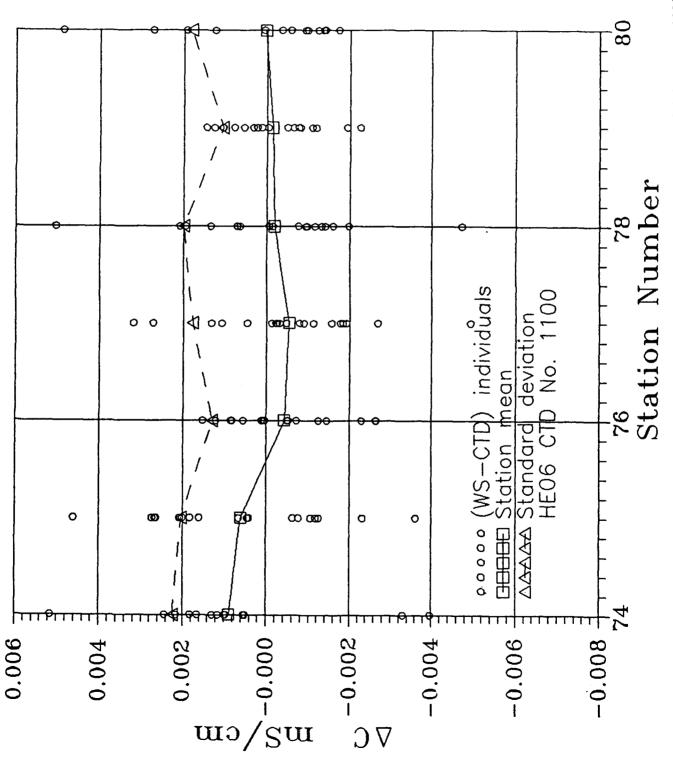


Figure 8: The conductivity residuals (water sample minus CTD) plotted versus station for Hesperides Cruise 6, July-August 1992, stations 74-80. The circles are the individual observations, the squares are station means, and triangles are the station standard deviation.

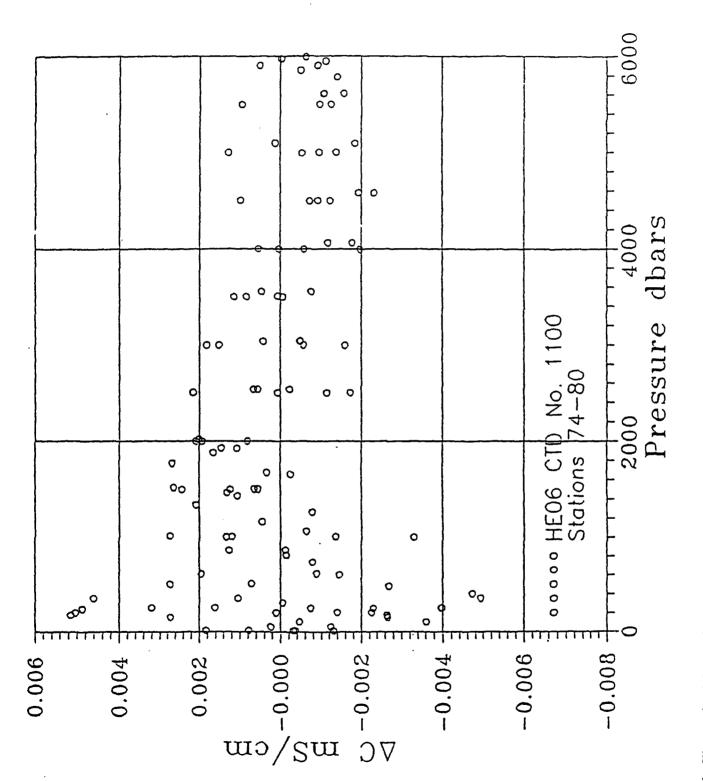
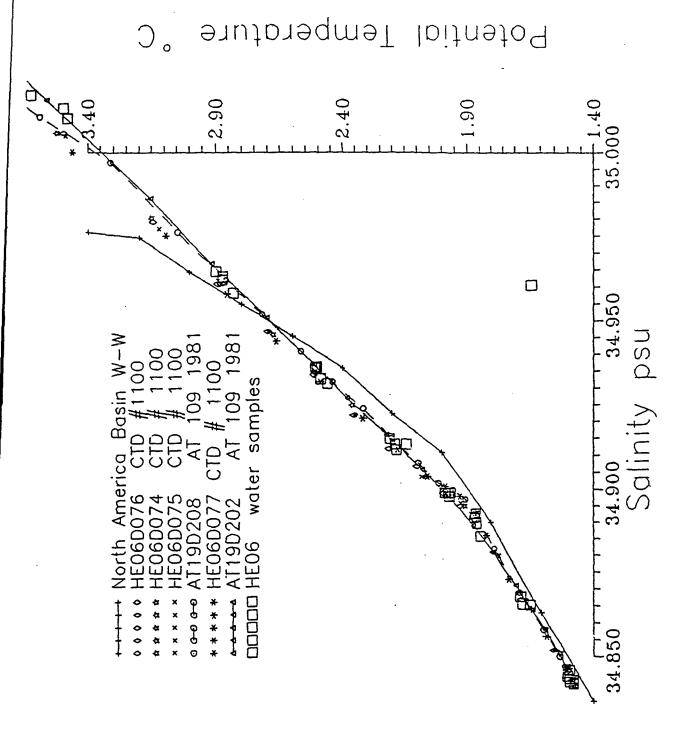


Figure 9: The conductivity residuals (water sample minus CTD) plotted versus pressure for BIO Hesperides Cruise 6, July-August 1992, stations 74-80. Note the reduction of scatter of residuals below 1000 decibars.



leg 3 and Worthington-Wright (1970) mean profile for the North America Basin are also included for comparison. Station 74 (stars) doesn't appear to be fresh when compared to neighboring stations 75, 76 or the Allantis stations from the same area 11 years earlier but both cruises appear to be Figure 10: A plot of CTD and water sample salinity versus potential temperature in the deep water below 3.5°C. Stations from Atlantis II cruise 109 resher than the Worthington-Wright profile based on IGY data of 1957.

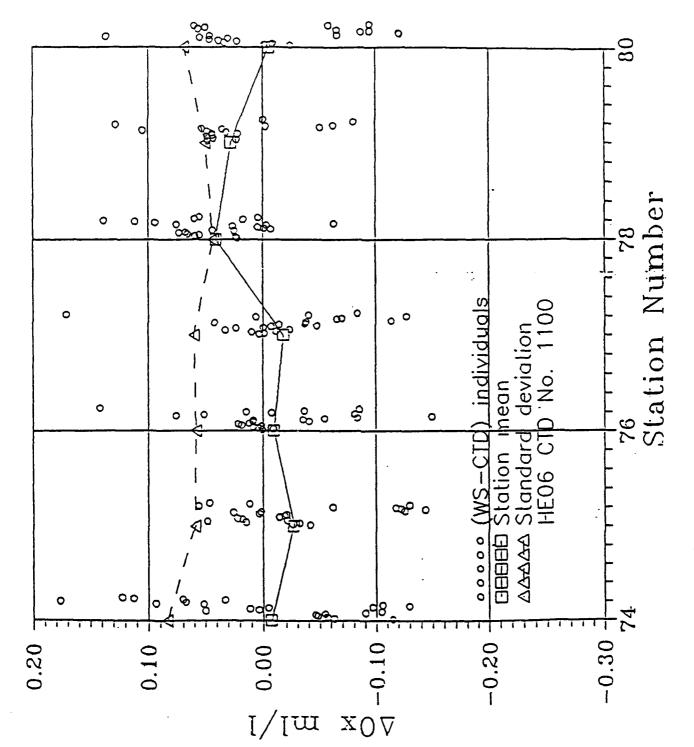


Figure 11: The oxygen residuals (water sample minus CTD) plotted versus station for BIO Hesperides Cruise 6, July-August 1992, stations 74-80. The circles are the individual observations, the squares are station means, and triangles are the station standard deviation.

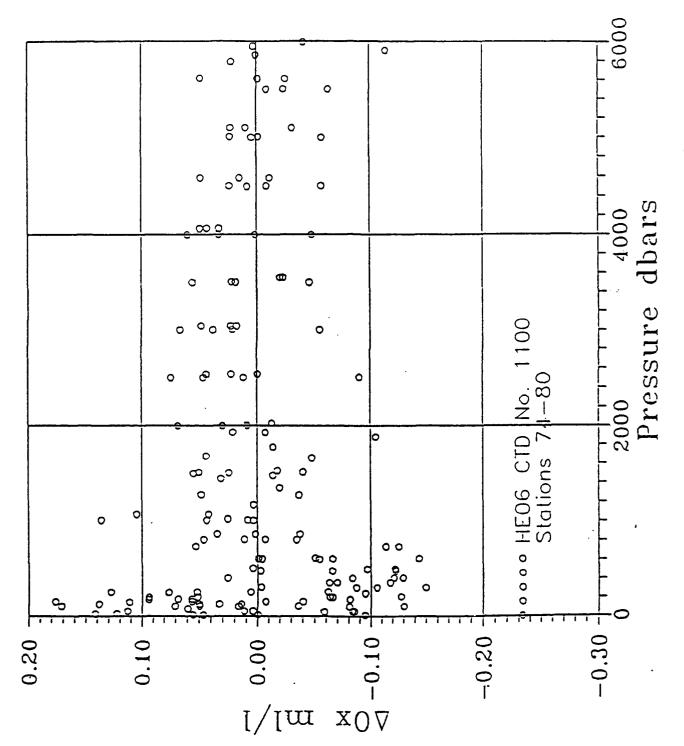


Figure 12: The oxygen residuals (water sample minus CTD) plotted versus pressure for BIO Hesperides Cruise 6, July-August 1992, stations 74-80. Again, note the reduction of scatter of residuals below 1000 decibars.

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16. Abstract (Limit: 200 words)

Processing methods, programs, and procedures currently used to create CTD data sets at Woods Hole Oceanographic Institution (WHOI) are described. The post-acquisition data processing steps include instrument calibrations in the laboratory and data calibration at sea, CTD data transformation from a time series to a pressure series, and the water sample data processing using the World Ocean Circulation Experiment (WOCE) format guidelines. Processing software has been developed for both the MicroVAX and IBM compatible personal computers. The description of the data processing procedures is restricted to the PC system. The programs are written primarily in FORTRAN with some format-related changes required between computer systems.

17. Document Analysis a. Descriptors

- 1. CTD calibration
- 2. CTD data processing methods
- 3. CTD processing programs
- b. Identifiers/Open-Ended Terms

c. COSATI Field/Group

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